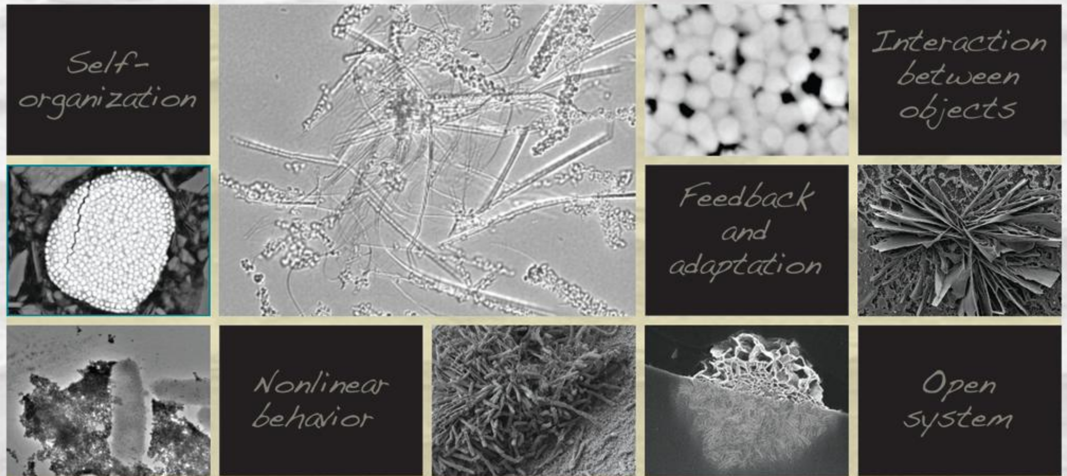
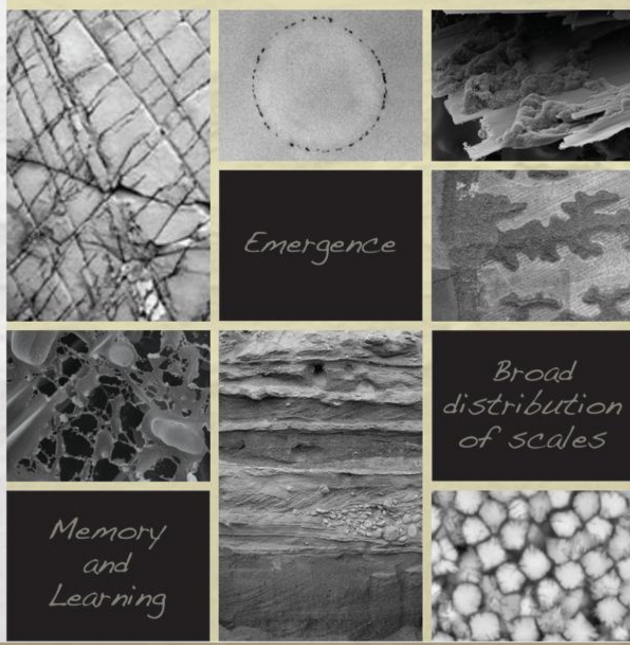
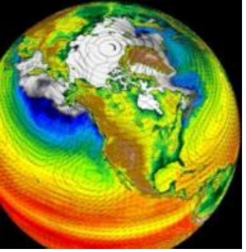
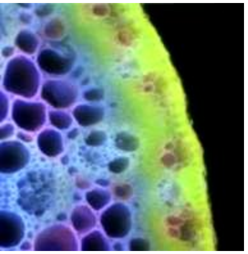
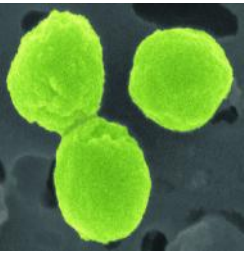


Complex Systems Science for Subsurface Fate and Transport



Report from the August 2009 workshop



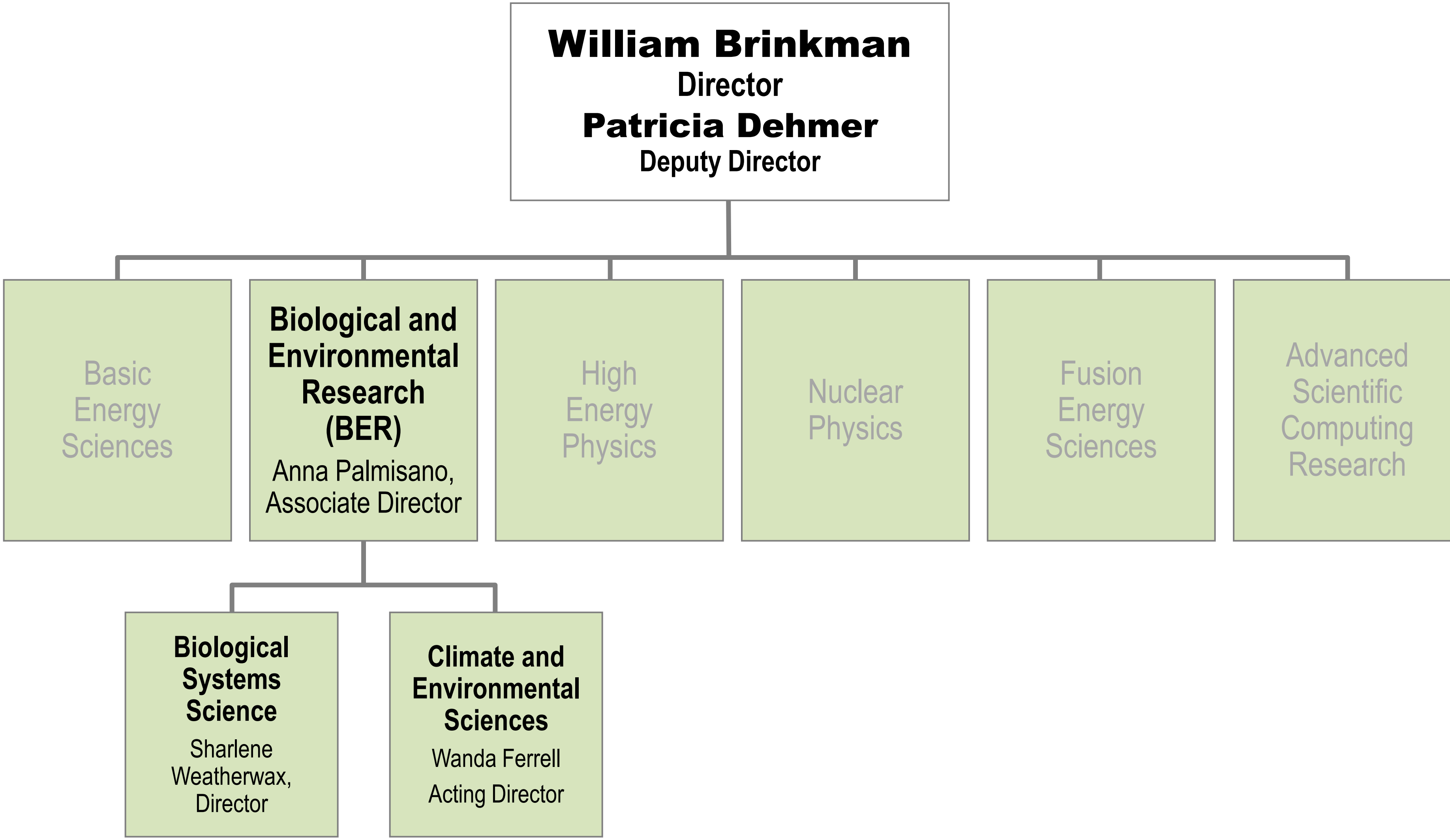
Subsurface Biogeochemical Research (SBR)

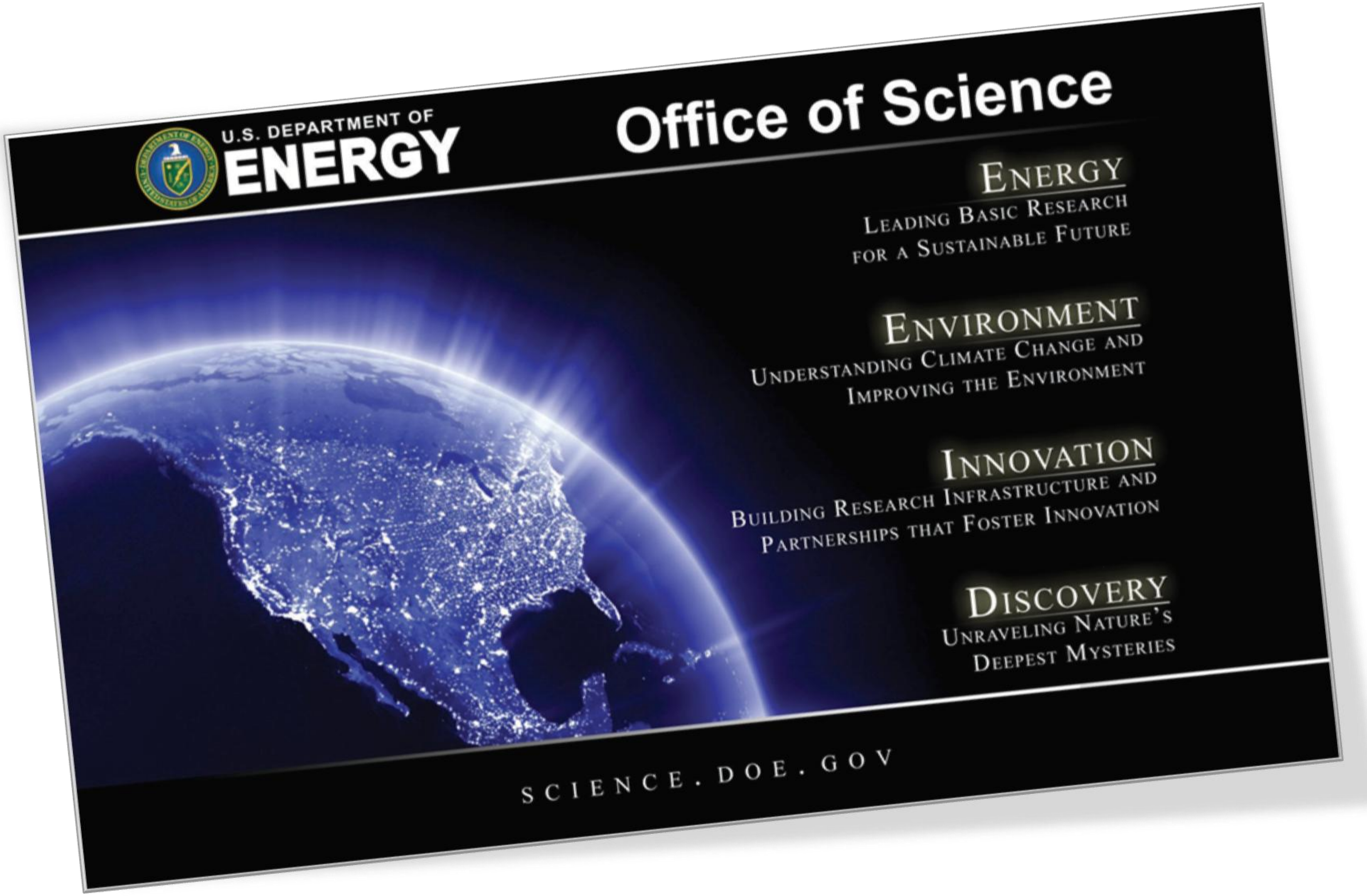
David Lesmes
Program Manager
Biological and Environmental Research

1. Overview of SBR: Goals and Approach
2. Strategic Plan & Complexity Workshop – August, 2009
3. SC-EM R&D Integration
4. Columbia River Corridor

    > 300 Area IFRC, SciDAC, Hyporheic Zone

Department of Energy Office of Science

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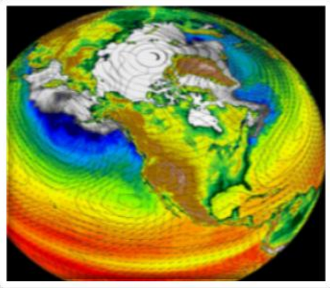
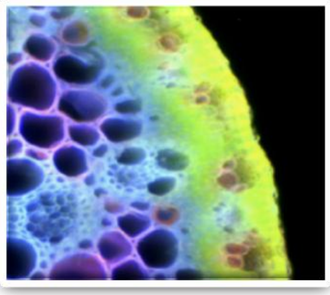
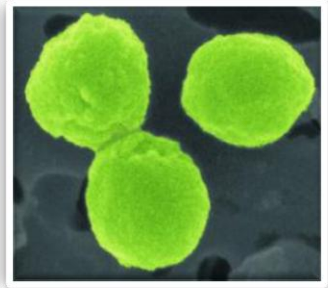
ENERGY
LEADING BASIC RESEARCH
FOR A SUSTAINABLE FUTURE
ENVIRONMENT
UNDERSTANDING CLIMATE CHANGE AND
IMPROVING THE ENVIRONMENT
INNOVATION
BUILDING RESEARCH INFRASTRUCTURE AND
PARTNERSHIPS THAT FOSTER INNOVATION
DISCOVERY
UNRAVELING NATURE'S
DEEPEST MYSTERIES
SCIENCE.DOE.GOV

Biological and Environmental Research Mission

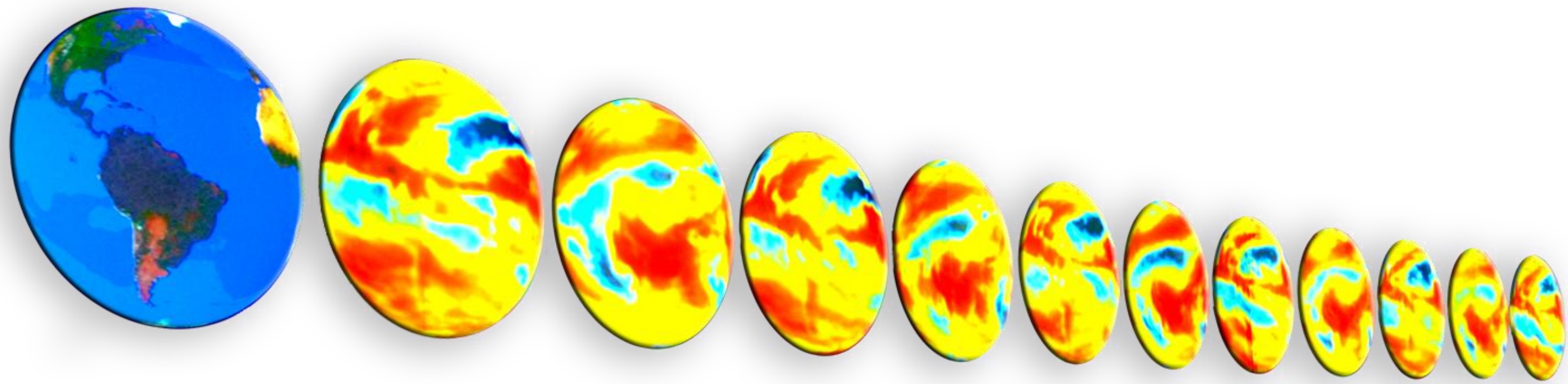
- To understand complex biological, climatic, and environmental systems across spatial and temporal scales.
- BER provides the foundational science to:
  - Support the development of next generation biofuels
  - Understand and predict the potential effects of greenhouse gas emissions on Earth's climate and biosphere – the energy-climate nexus
  - **Understand and predict processes in subsurface environments**
  - Develop new tools to explore the interface of biological and physical sciences

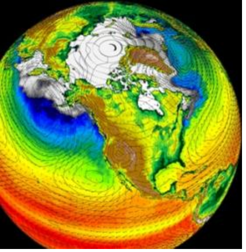


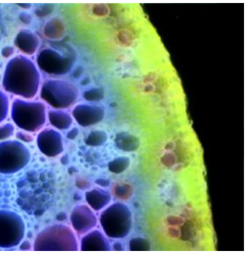
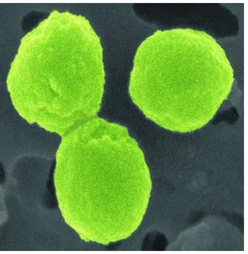




Biological and Environmental Research Approach

- Understanding complex biological and environmental systems across many spatial and temporal scales:
  - From the sub-micron to the global
  - From individual molecules to ecosystems
  - From nanoseconds to millennia
- **Integrating science by tightly coupling theory, observations, experiments, models, and simulations => predictive understanding**
- Supporting interdisciplinary research to address critical national needs
- Engaging national laboratories, universities, and the private sector to generate the best possible science





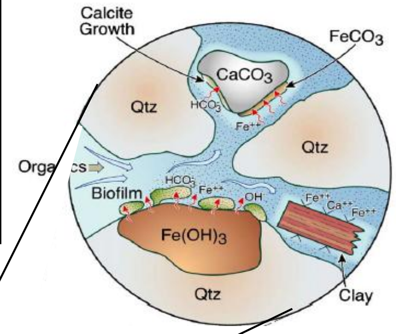




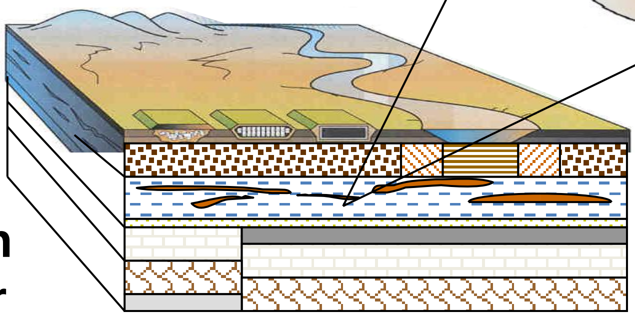
Subsurface Biogeochemical Research
($50M/yr)

Advancing a fundamental understanding of coupled physical, chemical and biological processes controlling contaminant mobility in the environment

Addressing DOE issues in intractable environmental remediation, long term stewardship and nuclear waste disposal


Oak Ridge field studies

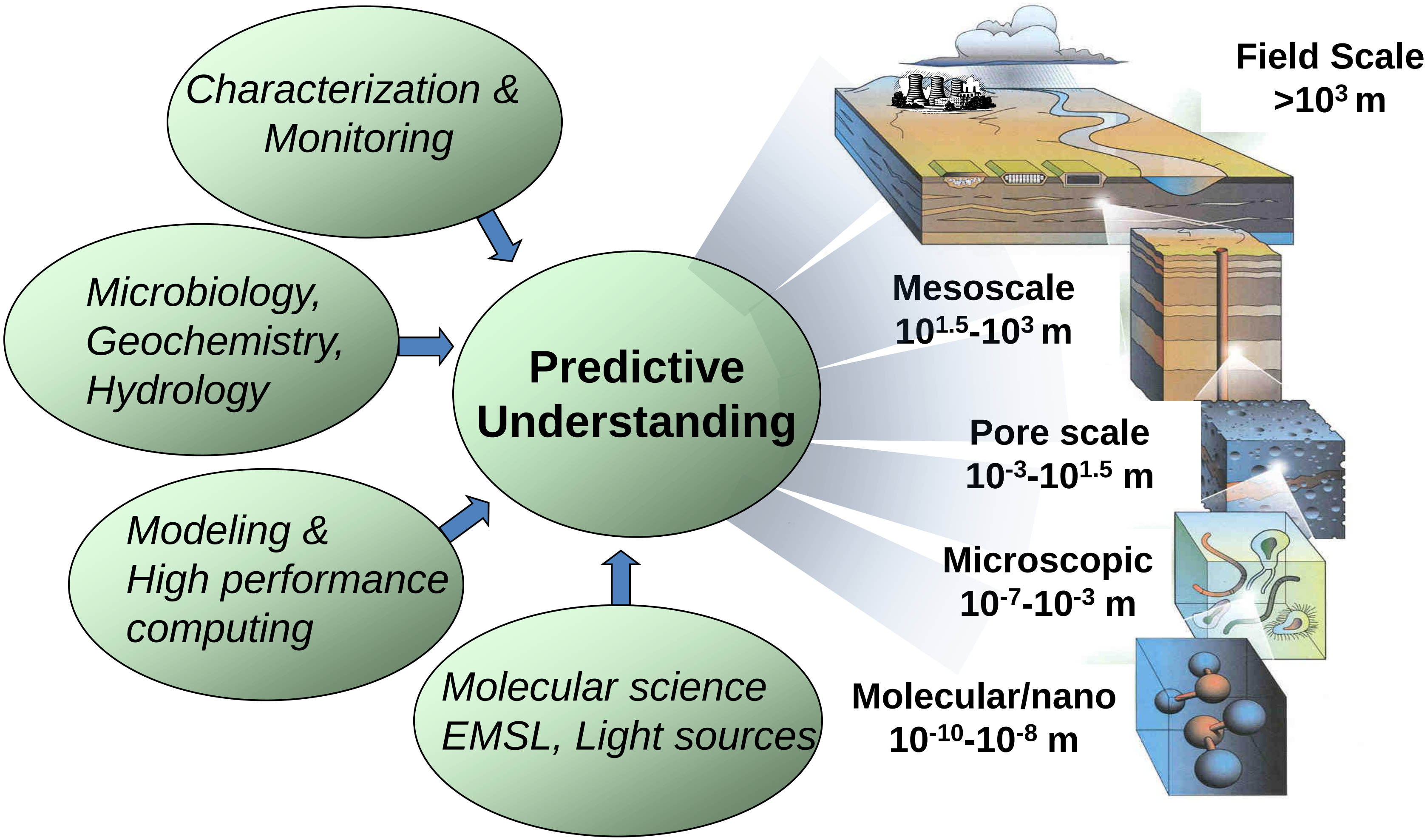




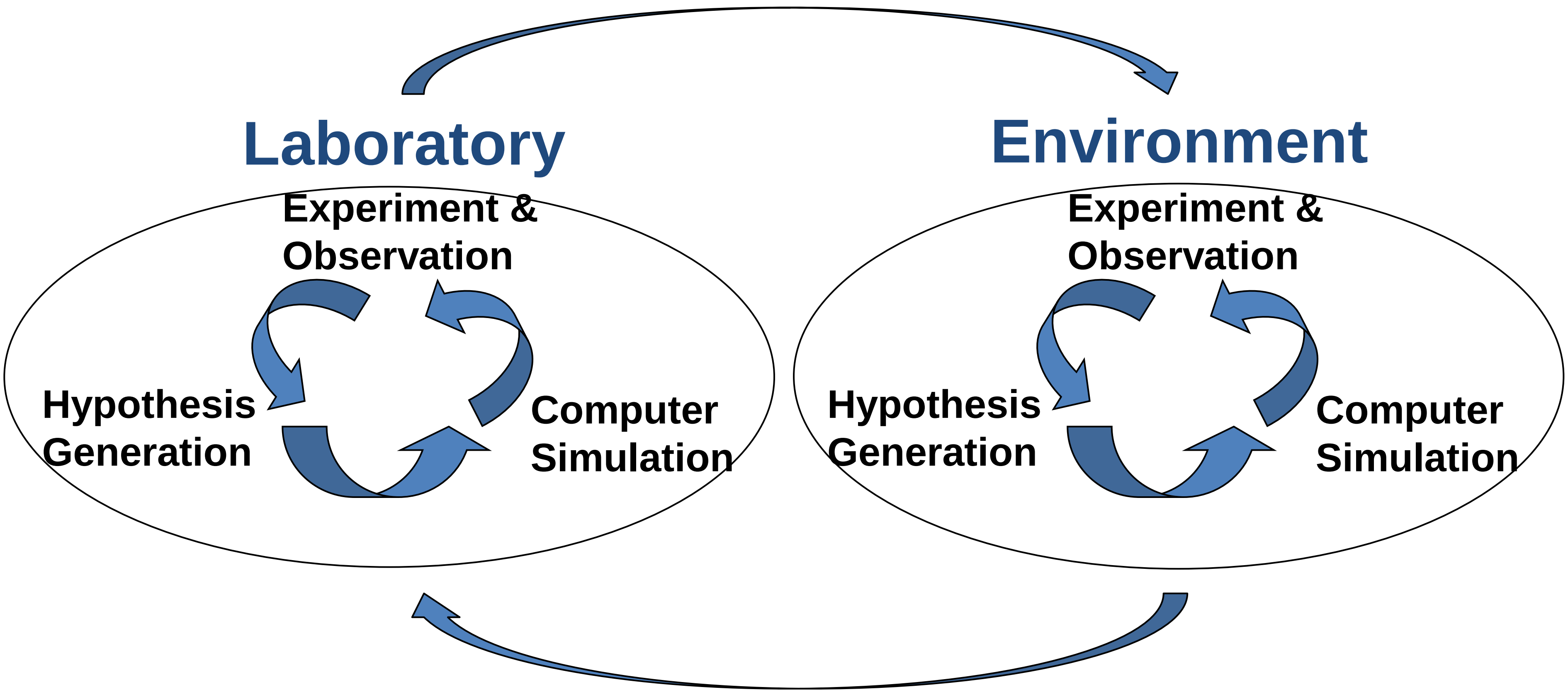
Current Contaminants of Concern
U, Tc, Pu, ^{90}Sr, ^{137}Cs, ^{237}Np, Hg, Cr

Subsurface Research Across Scales

Integrative, multidisciplinary approaches to understand multi-scale processes controlling contaminant mobility in the environment

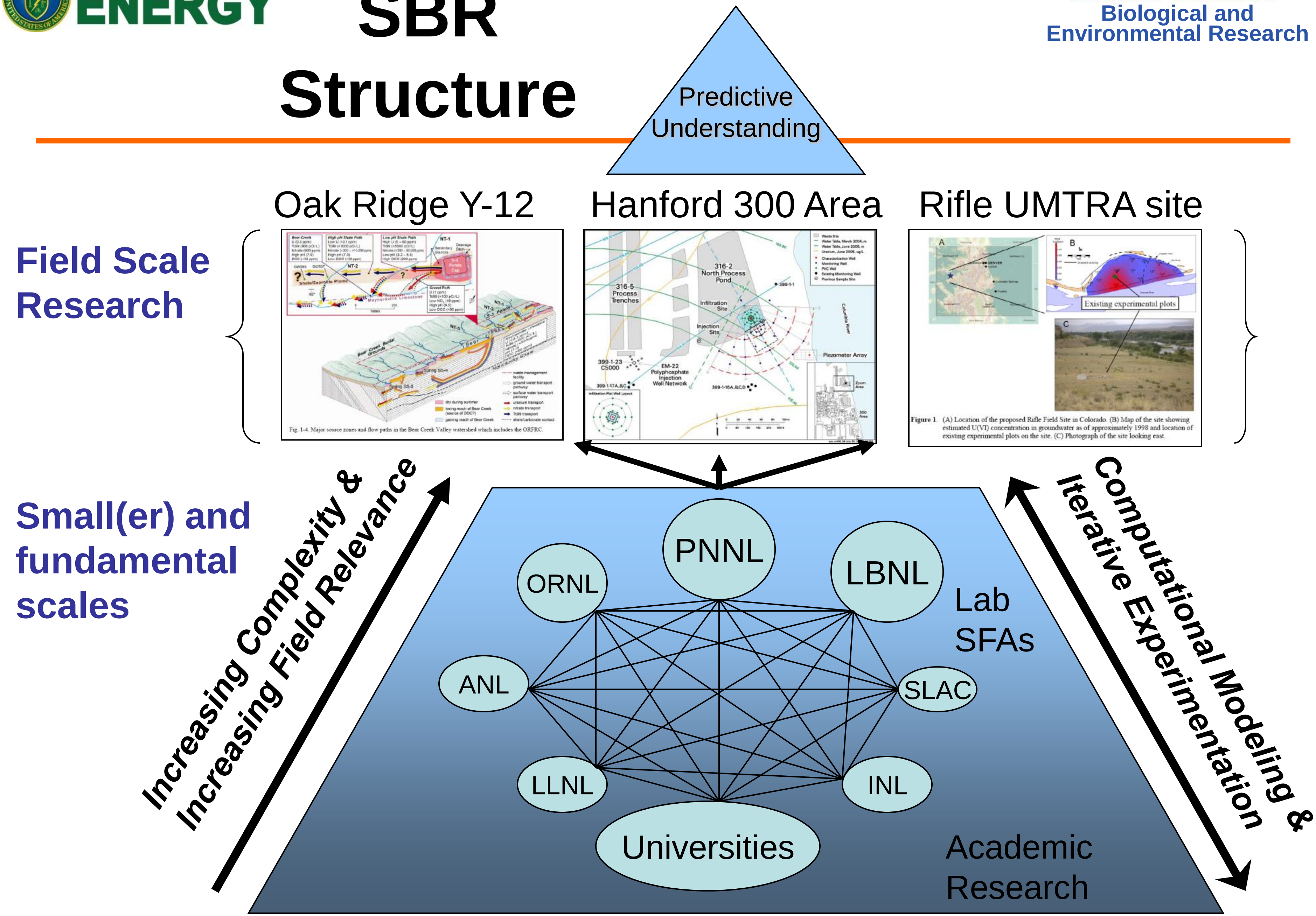


Iterative and Model Driven Investigations

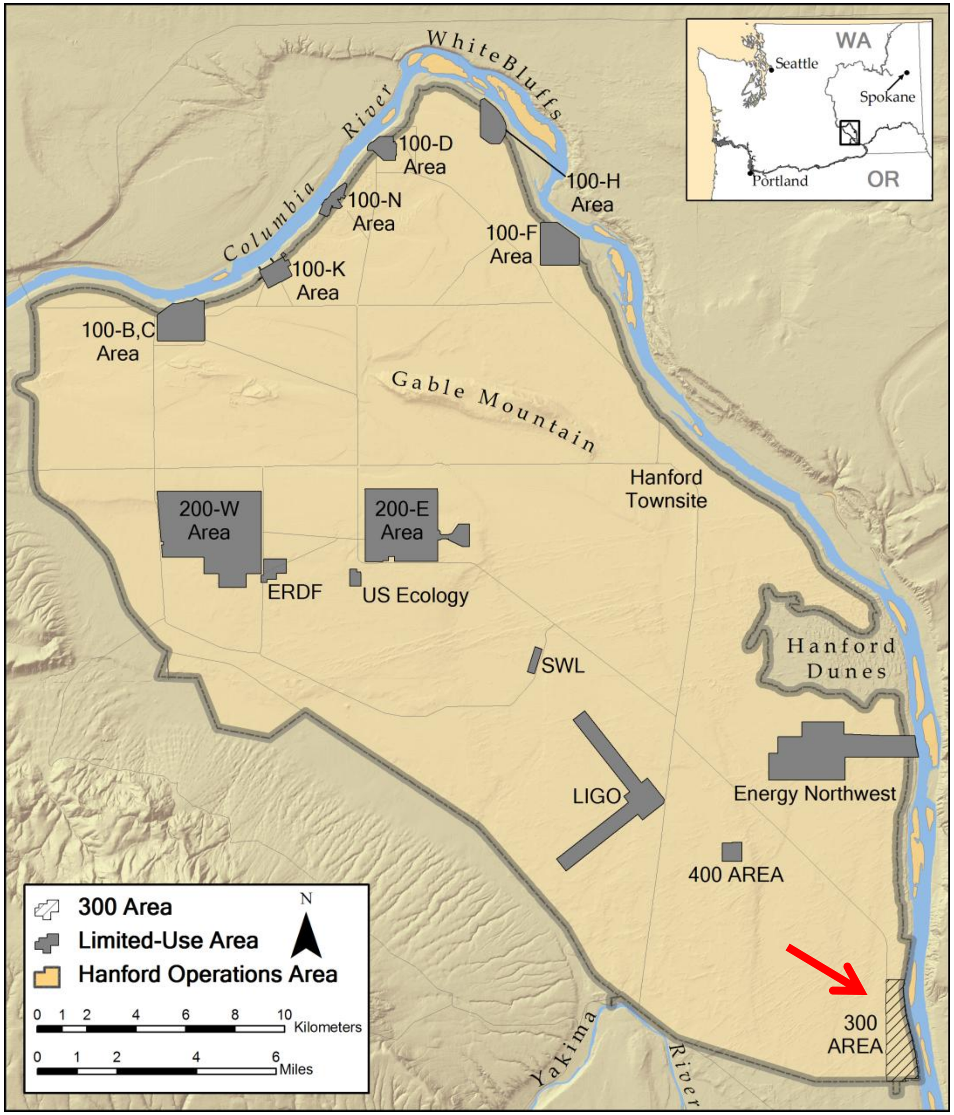


SBR seeks <u>predictive understanding</u> of the coupled processes controlling contaminant mobility in the environment. <u>Uncertainty</u> quantification/reduction and impact drive the decision making processes

SBR Structure



Hanford Site



Investigating In-Situ Mass Transfer Processes in a Groundwater U Plume Influenced by Groundwater-River Hydrologic and Geochemical Coupling

John M. Zachara and the IFRC Research Team

Pacific Northwest National Laboratory, Richland, WA

Supported by DOE-BER; Climate & Environmental Sciences Division (CESD); and Subsurface Environmental System Sciences Program (SESP)

AGU Meeting
December 15, 2009

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Environmental Remediation Sciences

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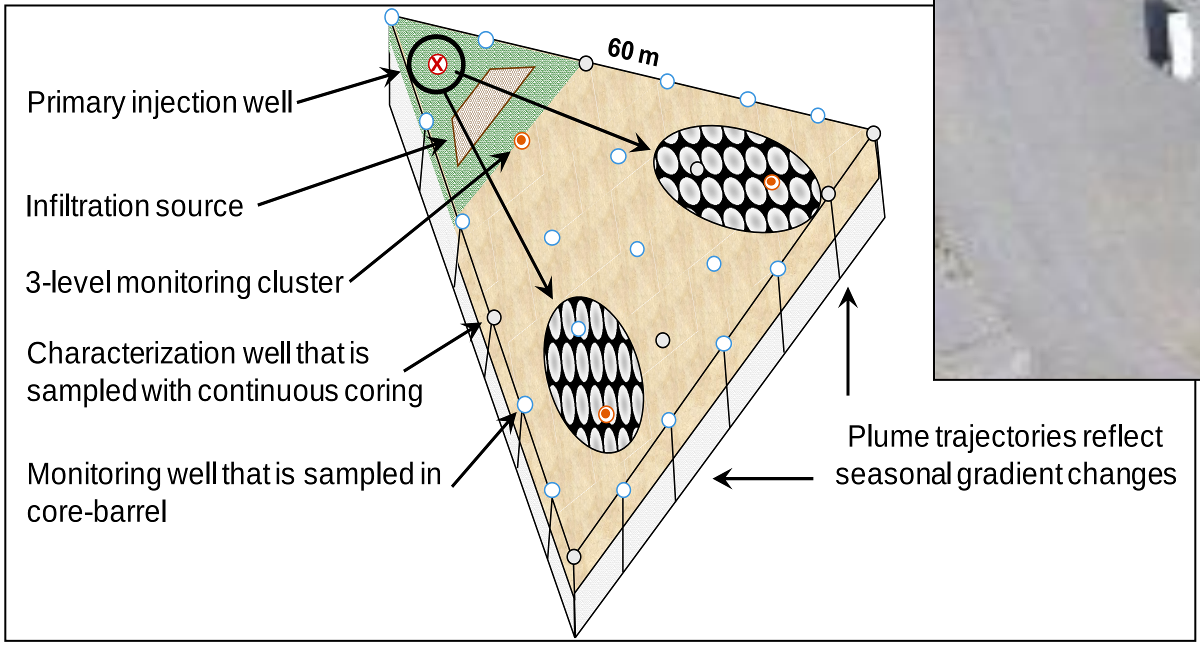
Hanford IFRC Site Concept



- Goal – Understand field scale factors controlling U(VI) plume dynamics with emphasis on mass transfer and GW-river coupling.
- Elements –
  - Robust field and laboratory characterization
  - Geostatistical models of physical, U, and geochemical reaction parameters
  - Field experiments to resolve global hypotheses
  - Development of a pragmatic reactive transport simulator including surface complexation and mass transfer
  - Documentation of system understanding through experiment-model iterations

Contaminant Transport at the Hanford Site:

Developing a Conceptual Framework for the Columbia River Corridor

BER Strategic Planning:

Contaminant Fate and Transport

Workshop report:
http://www.sc.doe.gov/ober/subsurfacecomplexity_03-05-10.pdf

Strategic plan:
http://www.sc.doe.gov/ober/Subsurface%20Biogeochemical%20Research%20Strategic%20Plan.pdf

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Developing a Plan

- Conduct workshop to Identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems

- Using the logic model format, develop a strategic plan for the BER contaminant fate and transport research program for a ten year planning horizon

    - Evaluate utilization of existing program elements and resources, consider needs

    - Consider points of integration with other BER mission areas and leveraging of other DOE research programs and facilities

    - Consider overarching BER complex systems science philosophy

The Logic of Logic Models

Contaminant Fate and Transport					
2	3	6	5	4	1
Current Situation	**Inputs / Resources**	**Near Term Goals (1-5 years)**	**Mid Term Goals (5-10 years)**	**Long Term Goals (10-15 years)**	**Outcomes (Impacts on science and society)**
Inadequate understanding of the *key* biogeochemical and hydrodynamic processes which control contaminant fate and transport in the environment Linear engineering approach does not account for the inherent complexity of real earth systems which leads to ineffective approaches to site characterization, modeling and management/stewardship	Integrated SFA research programs Engaged university research community with multidisciplinary capabilities Integrated Field Research Challenge (IFRC) sites EMSL, JGI, SciDAC, BES Geosciences, BES User Facilites EM, LM, USGS	Goal 1 Goal 2 Goal 3 	Goal 1 Goal 2 Goal 3 	Goal 1 Goal 2 Goal 3 	Improved understanding of contaminant transport and transformation through iterative, and interdisciplinary, experimentation and modeling. Improved management of the impacts of environmental contamination from past nuclear weapons production and the long-term stewardship of nuclear waste Reduced risks to human health and the environment.

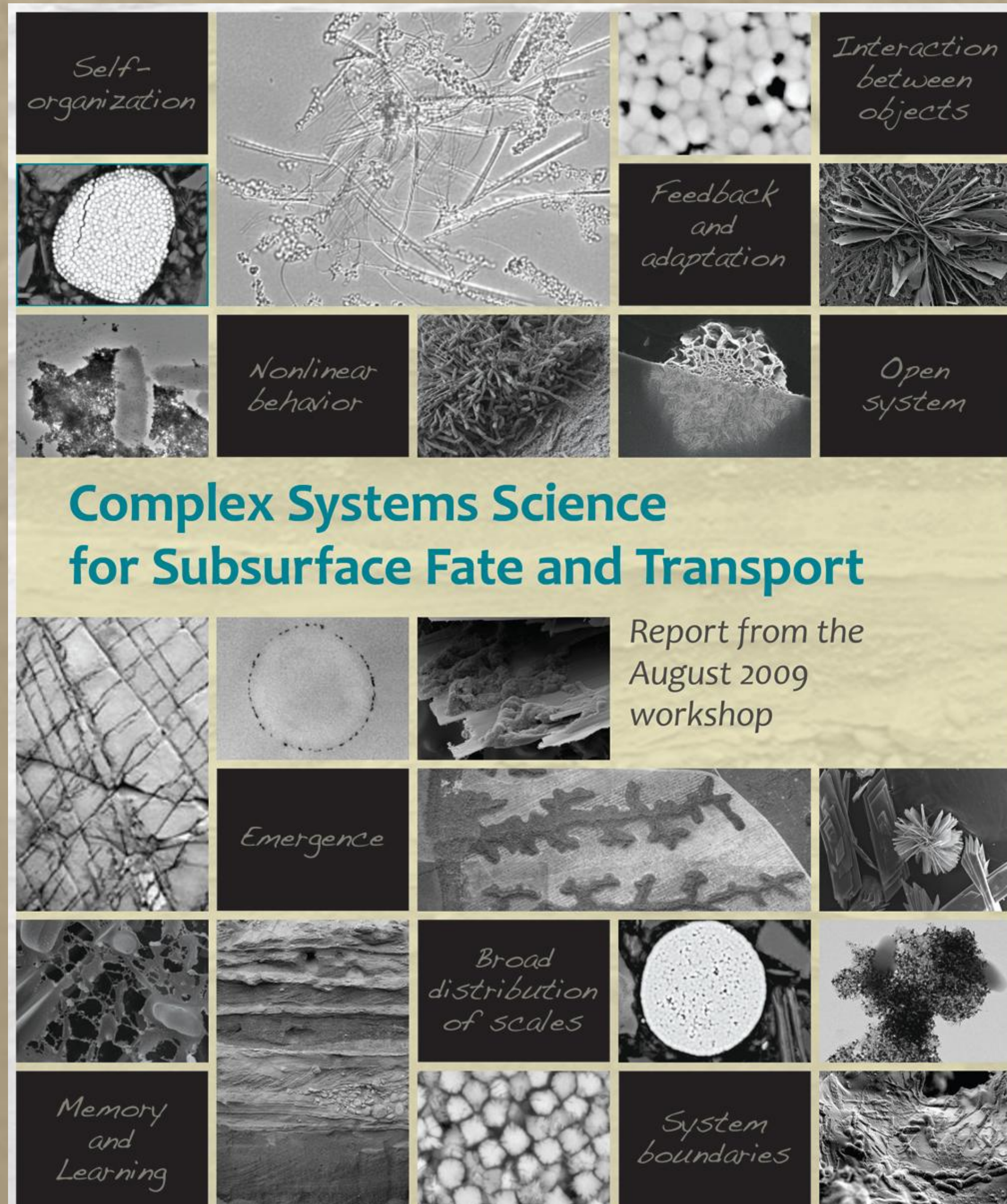
Desired Outcomes

- Increased understanding of coupled biogeochemical processes in key subsurface environments that enable system-level prediction and control.

- Robust strategies to monitor, immobilize or remove former weapons production-related contaminants from the environment.

- Science-based approaches to risk assessments of spent nuclear fuel storage.

- Societal Benefits: reduce the risk and cost of managing subsurface environmental and energy systems and increase public acceptance.


Self-organization
Interaction between objects
Feedback and adaptation
Nonlinear behavior
Open system

Complex Systems Science for Subsurface Fate and Transport

Report from the August 2009 workshop

Emergence
Broad distribution of scales
Memory and Learning
System boundaries

DOE-BER Workshop

Complex System Science for Subsurface Fate and Transport

Workshop Co-Chairs

Frank Loeffler — Georgia Tech

John Zachara — Pacific Northwest National Laboratory

Susan Hubbard — Berkeley Lab

Workshop Goal and Objectives

Goal – *Identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems*

Objectives:

- ***Define complex subsurface systems*** and establish why they are important to different DOE environmental and energy mission outcomes
- Consider how the ***coupling of subsurface processes (***hydrological, microbiological, and geochemical) defines complex system response and dynamics
- Evaluate ***research approaches*** that can be used to identify and account for the influence of smaller scale processes and their mechanisms on larger scale system behavior.
- Conceptualize models needed to describe and ***predict complex system behavior*** at different scales.
- Identify significant, long-term, ***interdisciplinary research opportunities*** associated with complex subsurface systems.

Workshop Discussion

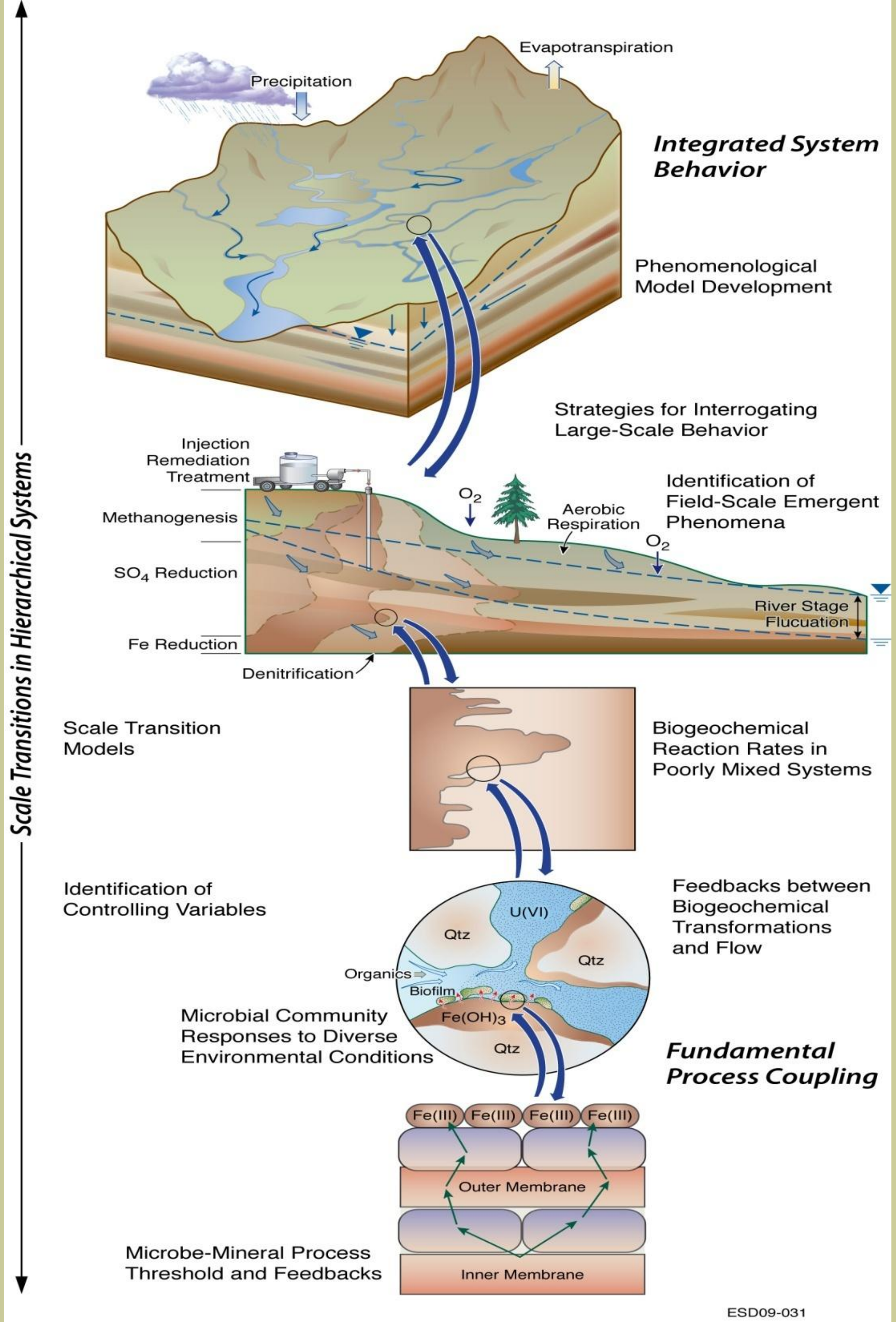
	Reductionism	Complexity
Philosophy	Overall system behavior can be understood from a detailed understanding of the system components	"More is Different" =>Emergence Seek to indentify and understand commonalities between complex systems and their relationship to more simple systems
Strategy	Understand and model system behavior as some permutation of the sum of its lower scale parts – blame heterogeneity for shortcomings	Identify diagnostic variables and transferable macro-scale laws that define/describe high-level system behavior – blame entropy for short comings (P.V.)
Research Approach	Bottom-Up: mechanistic	Top-Down: phenomenological
Modeling	Mechanistic details of lower scale processes are preserved but streamlined in upscaling. Models are "calibrated" to account for the effects of	Phenomenological models are used to explain and describe key processes contributions, interactions, and properties that control system behavior

Hybrid Approach: Reductionism + Complexity

- A pragmatic melding of bottom-up and top-down approaches.
- Emphasize the identification and understanding of *key* underlying mechanisms and interactions, and the importance of scale transitions, while simultaneously providing insights on common macroscopic laws governing complex system behavior at the prediction scale
- Goal is to achieve comprehensive and quantitative system predictability through iterative experimentation and modeling.

Complex System Research Opportunities

Research Opportunity	Challenge
1. Understand Fundamental Subsurface Process Coupling.	Coupled Mineral-Microbe Interfacial Processes
	Microbial Community Responses in Dynamic Subsurface Conditions
	Biogeochemcial Rates in Heterogeneous Media
	Feedbacks Between Biogeochemical Transformations and Flow
2. Identify and Quantify Scale Transitions in Hierarchical Subsurface Systems	Measurement Approaches for Key Variables and Diagnostic Signatures
	Identification of Smaller-Scale Controlling Variables
	Scale Transition Models
3. Understand Integrated Subsurface System Behavior	Identification of Field-Scale Emergent Phenomena
	Strategies for Interrogating Large-Scale Behavior
	Phenomenological Models for Prediction


Scale Transitions in Hierarchical Systems
Evapotranspiration
Precipitation
Integrated System Behavior
Phenomenological Model Development
Strategies for Interrogating Large-Scale Behavior
Injection Remediation Treatment
Identification of Field-Scale Emergent Phenomena
O_2
Aerobic Respiration
Methanogenesis
SO_4 Reduction
River Stage Flucuation
Fe Reduction
Denitrification
Scale Transition Models
Biogeochemical Reaction Rates in Poorly Mixed Systems
Identification of Controlling Variables
Feedbacks between Biogeochemical Transformations and Flow
U(VI)
Qtz
Organics
Biofilm
$Fe(OH)_3$
Microbial Community Responses to Diverse Environmental Conditions
Fundamental Process Coupling
Fe(III)
Outer Membrane
Inner Membrane
Microbe-Mineral Process Threshold and Feedbacks
ESD09-031

Summary and Workshop Findings

- **Apply a hybrid research approach** to advance predictive understanding of hierarchical subsurface systems by combining complimentary bottom-up reductionism with top-down complexity concepts through **iterative experimentation and modeling**.
- Focus well-conceived, hybrid research efforts at selected **DOE-relevent field study sites, and representative laboratory model systems** at different scales, that offer the most potential for understanding fundamental process interactions that occur across scales and lead to complex subsurface behavior.
- Explore the value of complex system science approaches in providing the scientific basis for effective DOE management of earth/environmental systems

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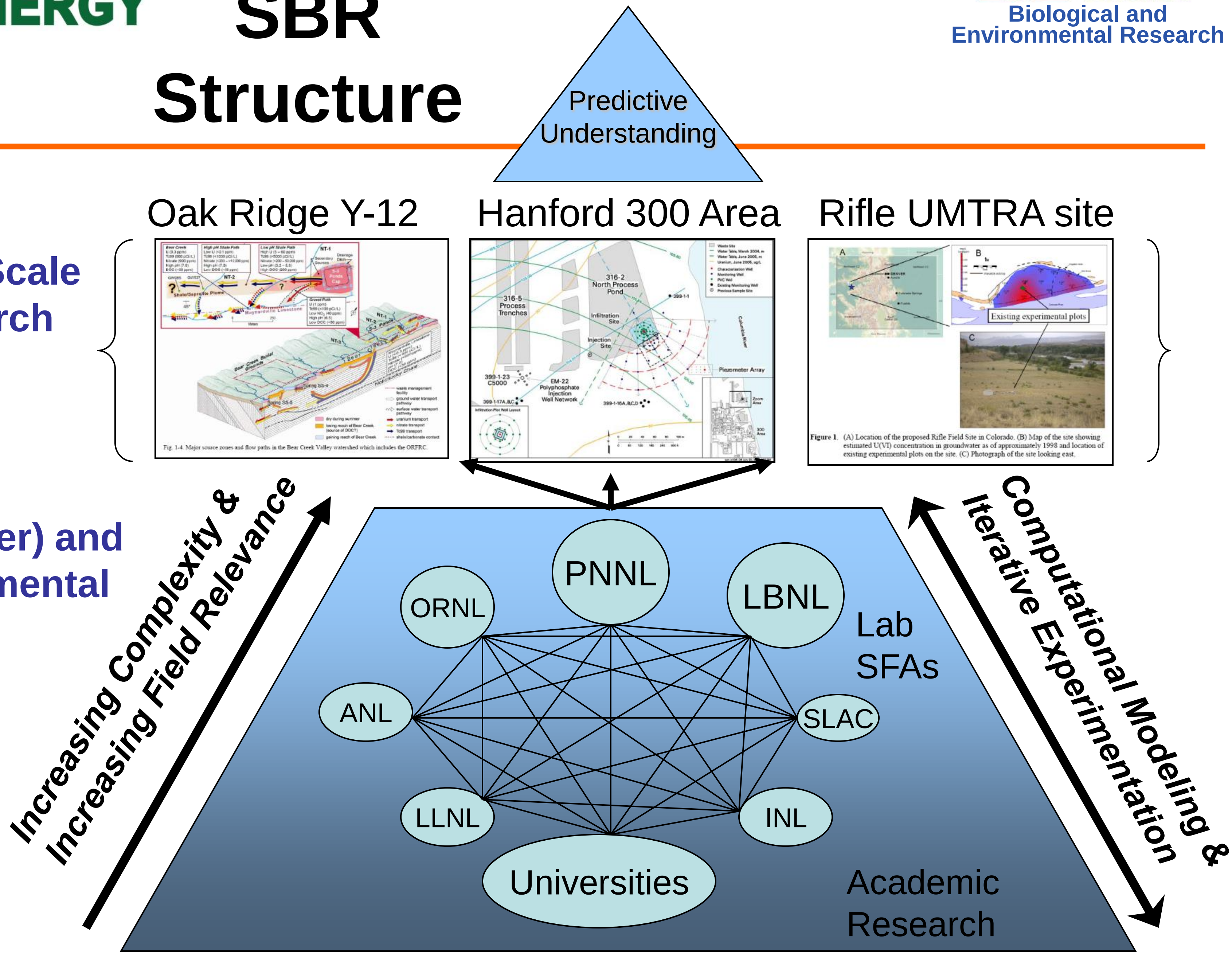
SBR Structure



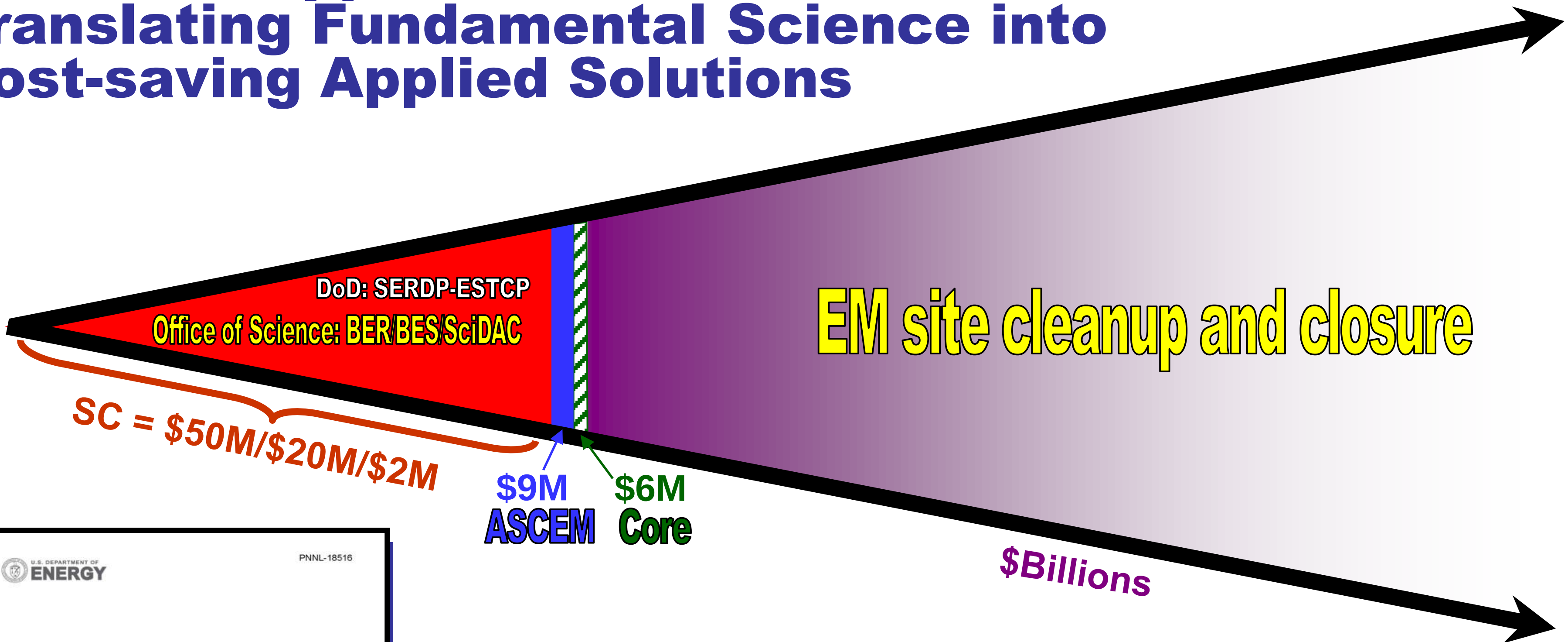
Field Scale Research

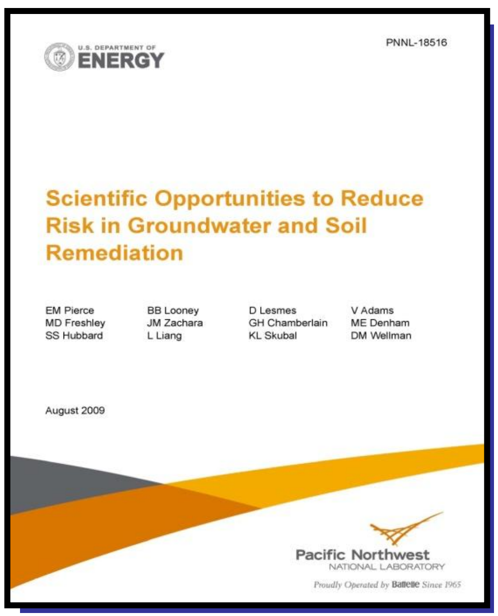
Small(er) and fundamental scales

Implications: R&D Integration and Solutions

- For complex systems, understanding just the components of the system does not provide predictive understanding of the complete system. “Scientists and science programs need to meaningfully engage with problems at relevant scales and sites” – Steve Koonin
- Although we strive to develop common principles and approaches, each site is unique and solutions/decisions need to be developed using a phased (iterative) approach that is science based (understand, predict, control, monitor => a “living model”) – Carol Eddy-Dilek
- Seek solutions that are robust to uncertainty – Brian Looney
- Effective solutions will require integrated and collaborative approaches involving basic and applied science, contractors and regulators. Linear approaches to remediation solutions are not effective.
- Prioritize efforts to focus on major risk drivers and holistic systems approaches to solutions

Scientific Opportunities to Reduce Remediation Risk: Translating Fundamental Science into Cost-saving Applied Solutions

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PNNL-18516

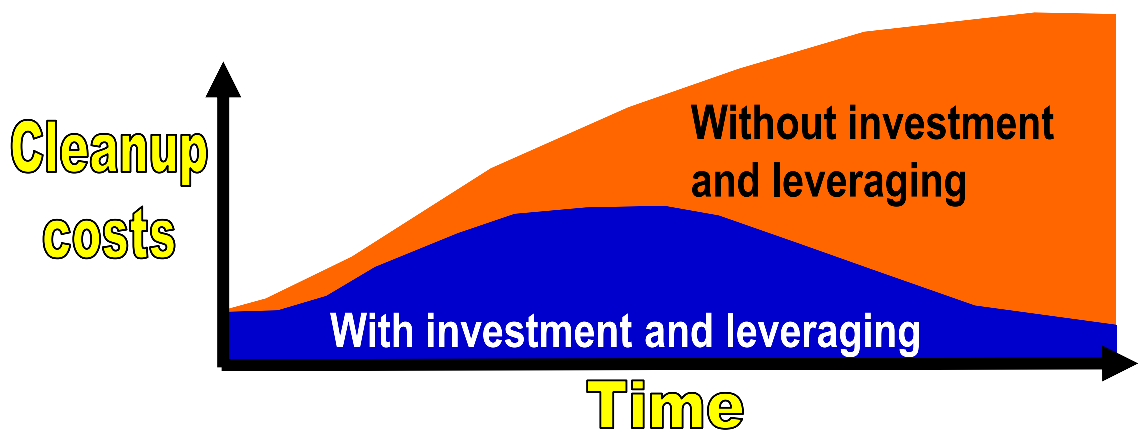
Scientific Opportunities to Reduce Risk in Groundwater and Soil Remediation

EM Pierce, MD Freshley, SS Hubbard, BB Looney, JM Zachara, L Liang, D Lesmes, GH Chamberlain, KL Skubal, V Adams, ME Denham, DM Wellman

August 2009

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965



Advanced Simulation Capability for Environmental Management

ASCEM Multi-Lab Program Manager
Paul Dixon

ASCEM

Presentation to Office of Technology Innovation and Development
3rd Quarter Review Meeting July 7-8, 2010

ASCEM National Laboratory Consortium

Berkeley Lab

Los Alamos National Laboratory
EST. 1943

Pacific Northwest National Laboratory

Oak Ridge National Laboratory

SRNL
Savannah River National Laboratory

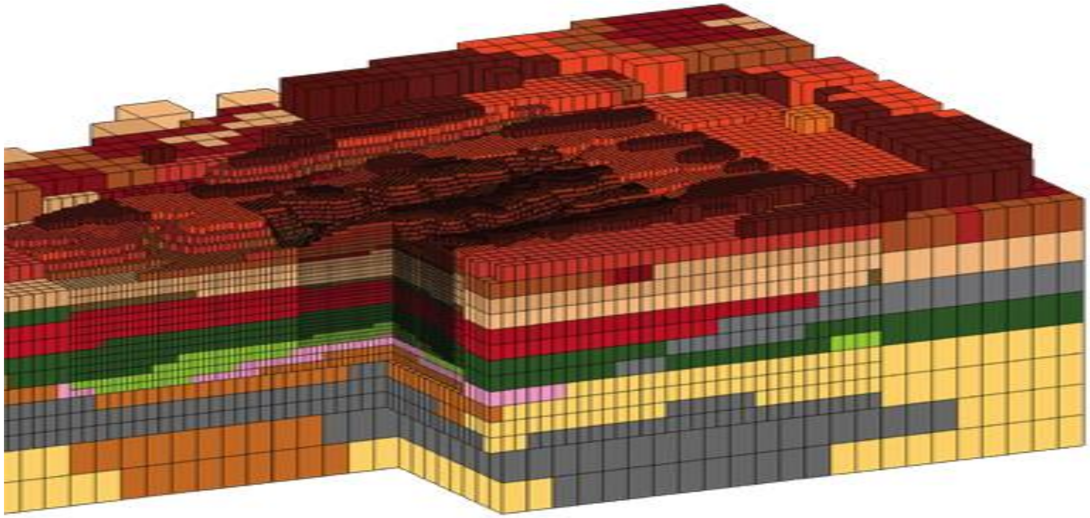
Lawrence Livermore National Laboratory
Science in the National Interest

Argonne National Laboratory

INL
Idaho National Laboratory

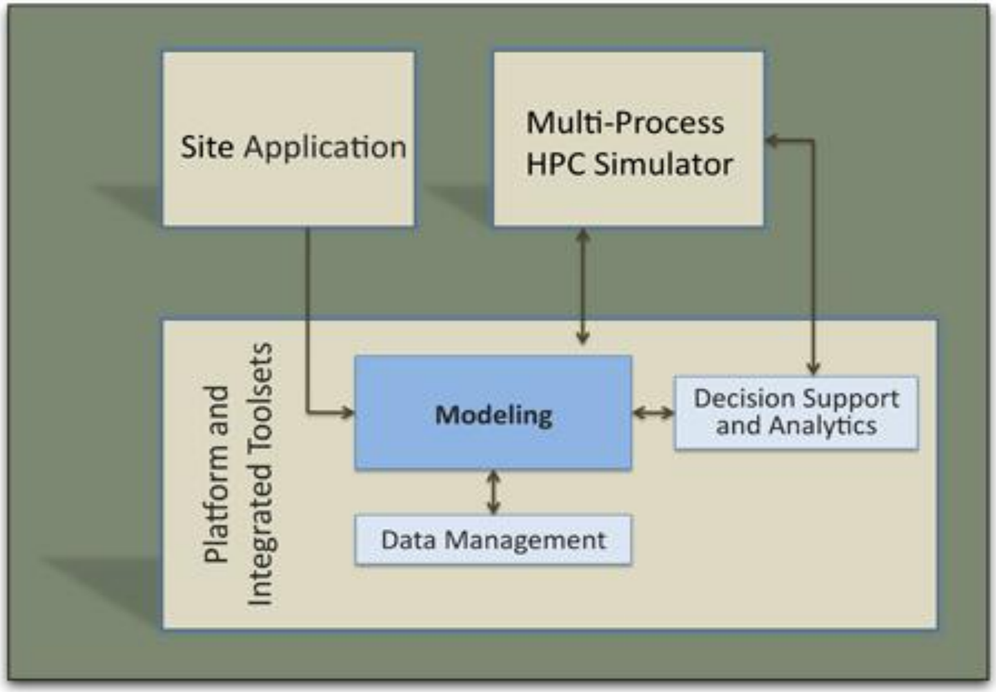
What is ASCEM?

ASCEM is a state-of-the-art ***scientific tool and approach*** *for understanding and predicting contaminant fate and transport in natural and engineered systems. ASCEM is a Modular and open source HPC tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized development of performance and risk assessments for EM cleanup/closure activities*.



ASCEM

ASCEM Overall Structure



- **Platform and Integrated Toolsets**
  - Facilitate model development and execution, parameter estimation, uncertainty quantification, decision support and risk analysis
- **Multi-Process High Performance Computing Simulator**
  - Modular simulation capability for barrier and waste form degradation, multiphase flow and reactive transport
- **Site Applications**
  - Demonstration sites
  - Actively engage site user community to develop and test ASCEM tools

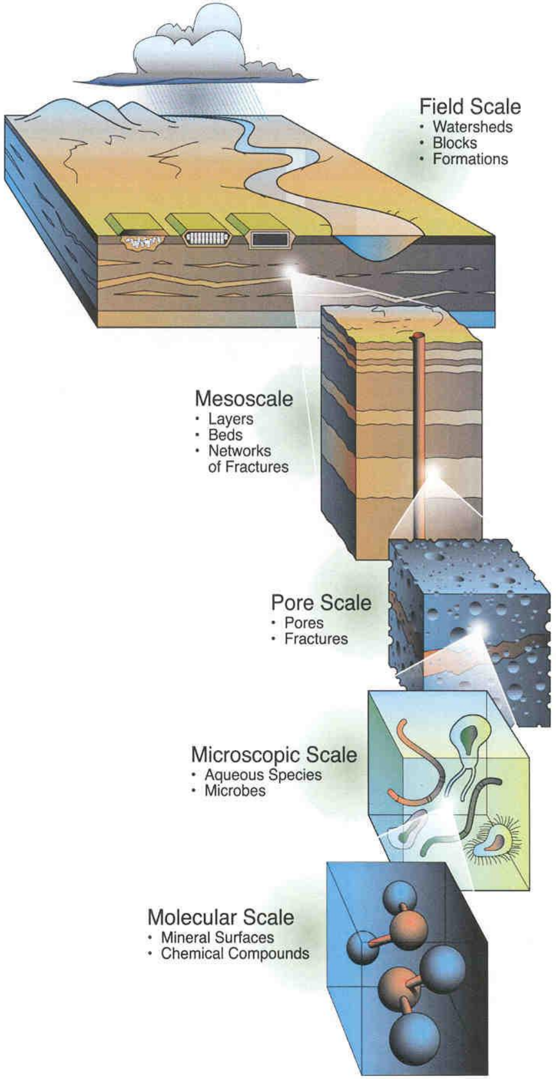
Summary

Office of Science

➢ SBR's challenge is to orient multidisciplinary DOE Laboratory programs and University-led projects towards iterative understanding of key processes affecting contaminant mobility in the environment to help provide DOE with science-based solutions (approaches) for its remaining (currently intractable) environmental problems.

➢ SC and EM Programs are working closely together to develop and strategically implement science based tools and approaches – building on established capabilities

➢Establishing credibility and confidence of regulators and stakeholders is critical. Must include them in the process. This is part of the ASCEM plan/approach.




Thank you!

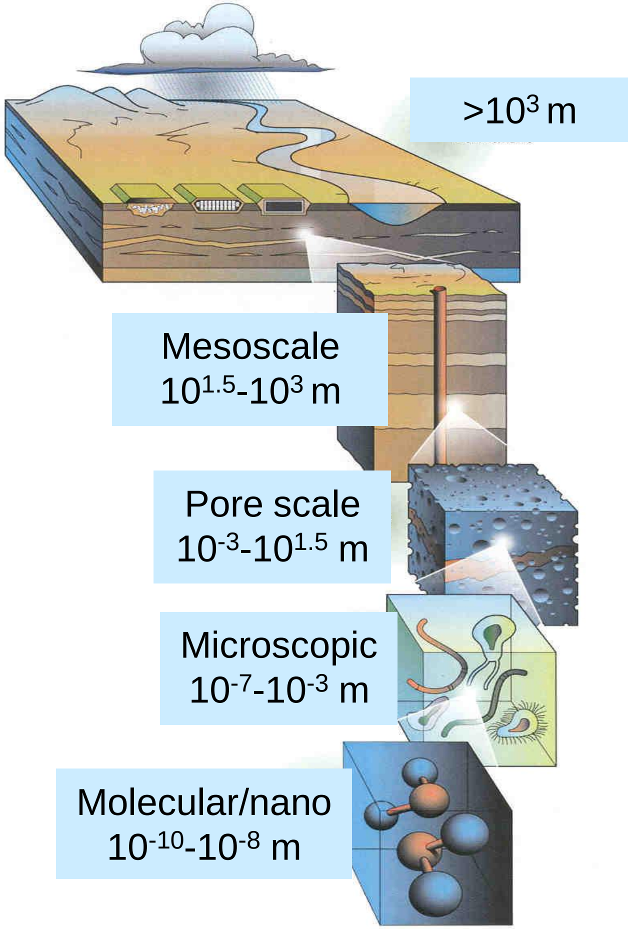
Scientific Focus Areas at the National Laboratories

Team-oriented Approach to Subsurface Science

PNNL ($6.5M) - Integrated investigations of geochemical, microbial and transport processes at different scales. Focus on Hanford Site (U, Tc, Pu)
LBNL ($4.5M) – Integrated investigations of geochemical, microbial and transport processes at different scales. Hanford 100 Area, Old Rifle IFRC, SRS F-Area (U, Cr, I)
ORNL ($3M) – Biogeochemistry, microbial processes (Hg)

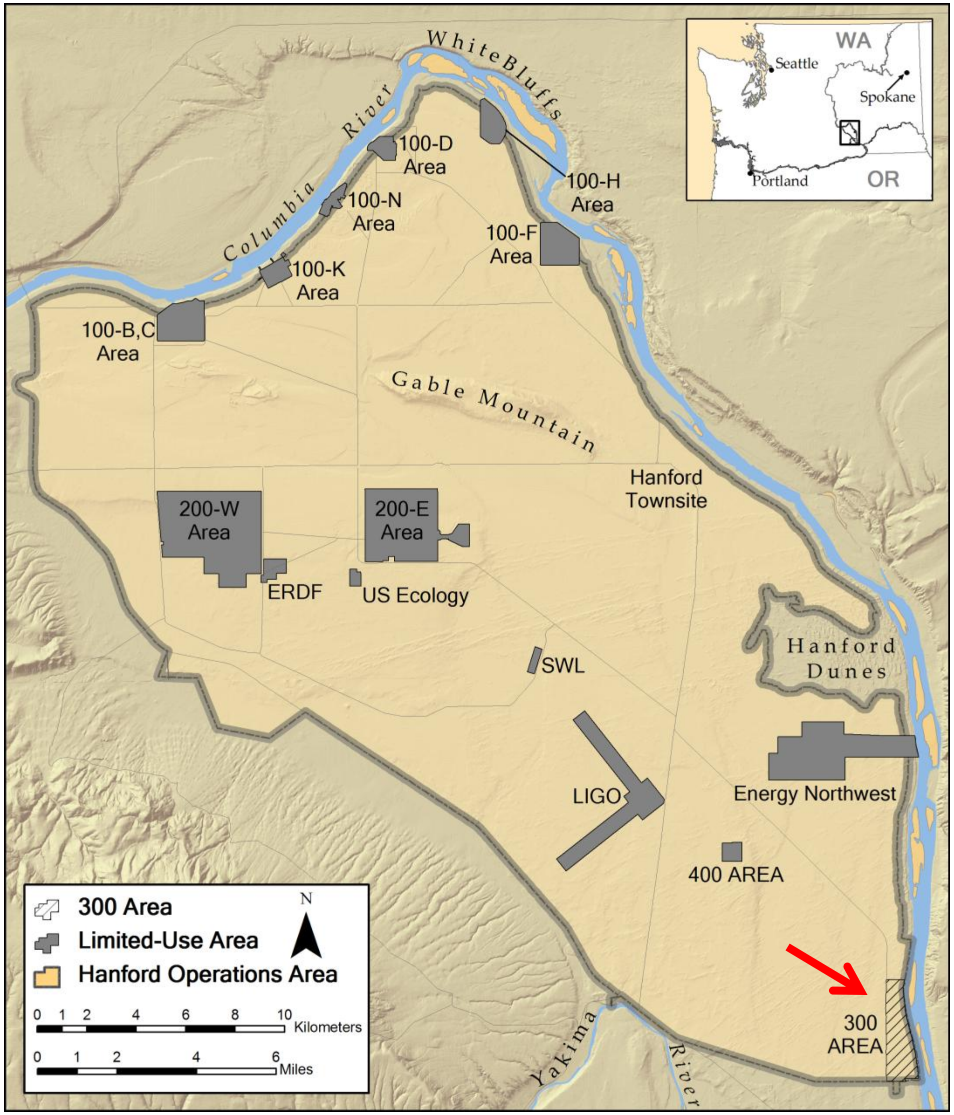
ANL ($1.5M) – Synchrotron environmental science
SLAC ($0.7M) – Synchrotron environmental science

LLNL ($1.2M) – Pu geochemistry at NTS – colloid transport
INL ($1.5M) – Immobilization of metal contaminants by amendment-driven mineral precipitation (Sr)



- ***Lab programs rigorously reviewed every three years***
- ***SFA Programs collaborative with the University community***

Hanford Site



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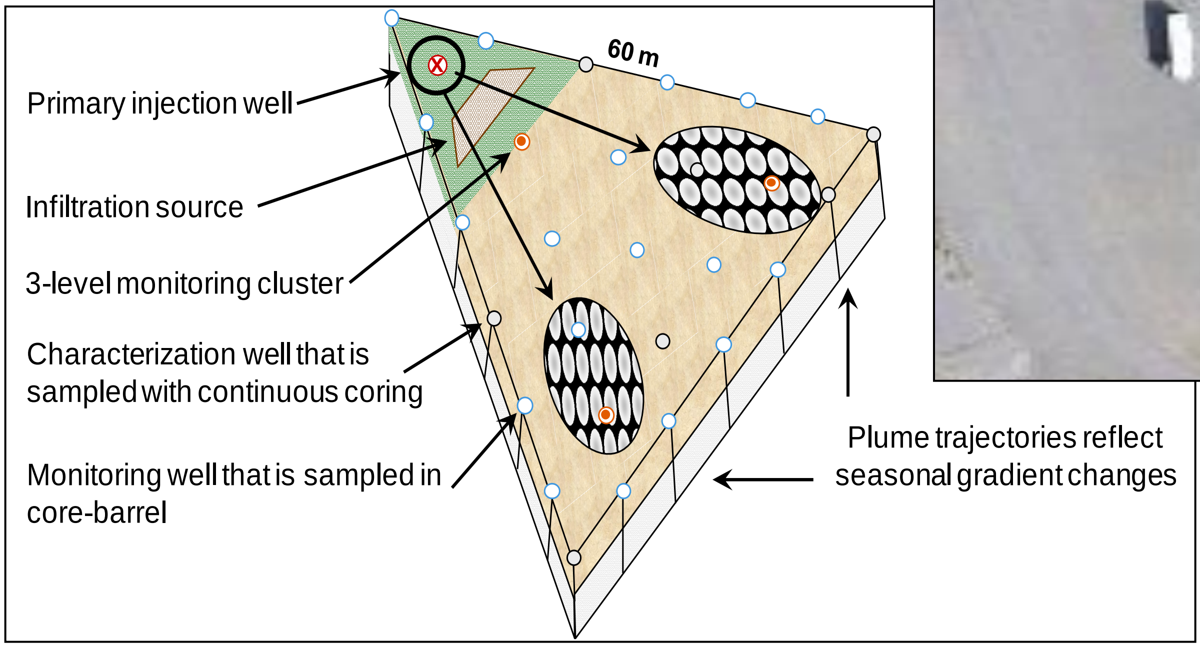

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  - Field experiments to resolve global hypotheses
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SciDAC : Scientific Discovery through Advanced Computing

SciDAC – A partnership between DOE's Office of Advanced Scientific Computing (ASCR) and the other Program Offices within the Office of Science (http://www.scidac.gov/).

- 5 –year projects
- teams application scientists with computational scientists
- explores the potential of using high performance computing to address DOE mission areas

ERSP Co-funds two SciDAC projects with ASCR

Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing (Lead PI: Peter Lichtner, LANL (https://software.lanl.gov/pflotran)

Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes (Lead PI: Tim Scheibe, PNNL (http://subsurface.pnl.gov/)

Mid-term review of SciDAC projects conducted in April 2009

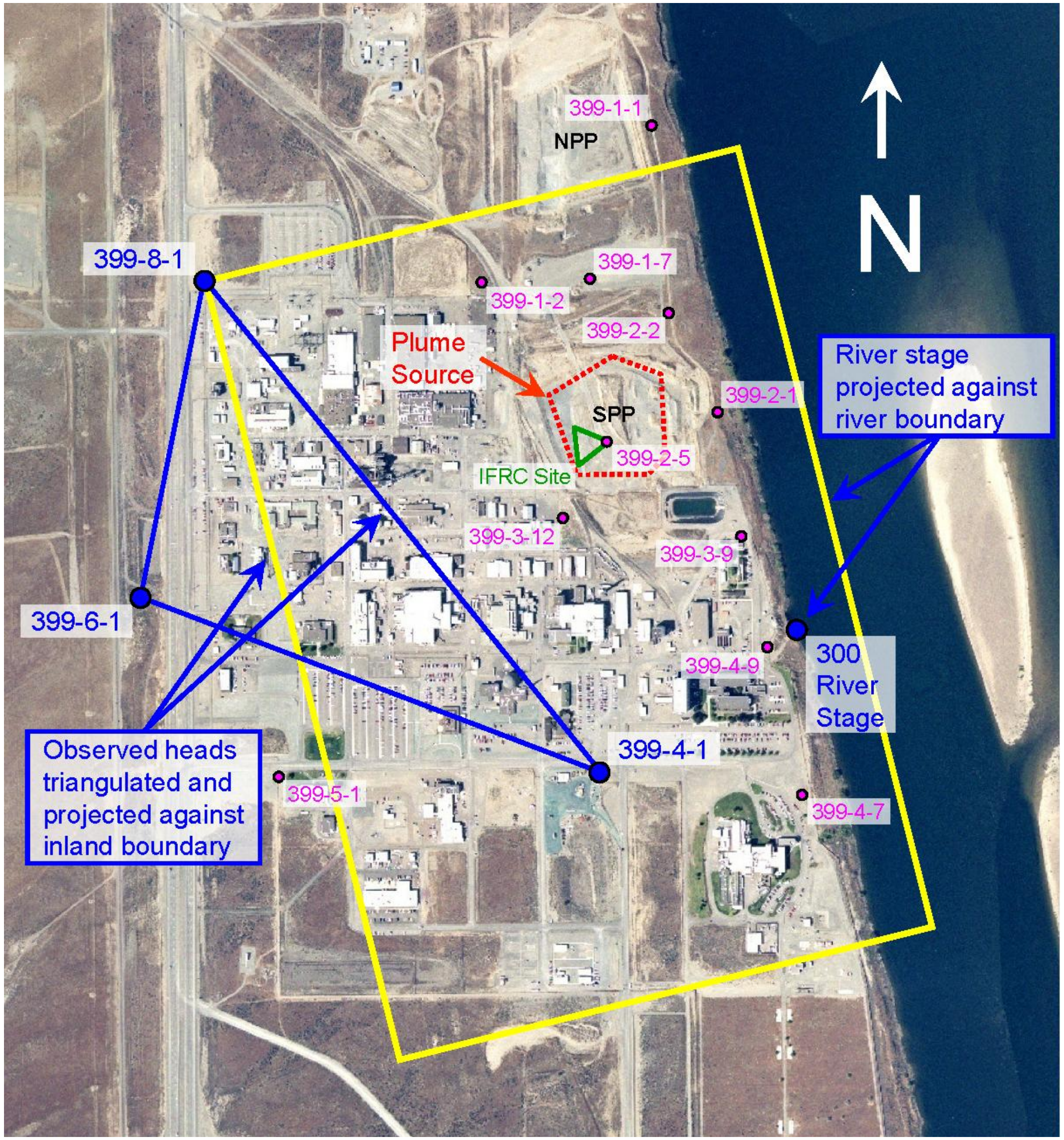
Placing the Hanford 300 Area IFRC Site in Perspective: Plume-scale Modeling of Uranium Attenuation and Its Flux to the Columbia River

SciDAC Research

P.C. Lichtner (PI), *LANL*; G. E. Hammond, *PNNL*; R. Milles, *ORNL*; D. Moulton, D. Svyatskiy, *LANL*;
B. Smith, *ANL*; A. Valocchi, *U. of Illinois at Urbana-Champaign*, B. Philip, *ORNL*

Hanford 300 Area Conceptual Model

- Problem domain:
  - 900×1300×20 meters
  - $\Delta x/\Delta y$ = 5 meters
  - Δz = 0.5 meters
  - 1.87M grid cells
  - 28M unknowns
- 1-year simulation:
  - '92-'93 (8pm Dec. 25)
  - Δt = 1 hour
- High Performance Computing
  - 4096 processor cores (single realization)
  - 40960 processor cores (10 realizations)
  - 6 - 12 hours runtime



RUTGERS
THE STATE UNIVERSITY OF NEW JERSEY

Hydraulic Characterization the Hyporheic Corridor at the Hanford 300 Area Using Geoelectrical Imaging and Distributed Temperature Sensing (DTS) Methods

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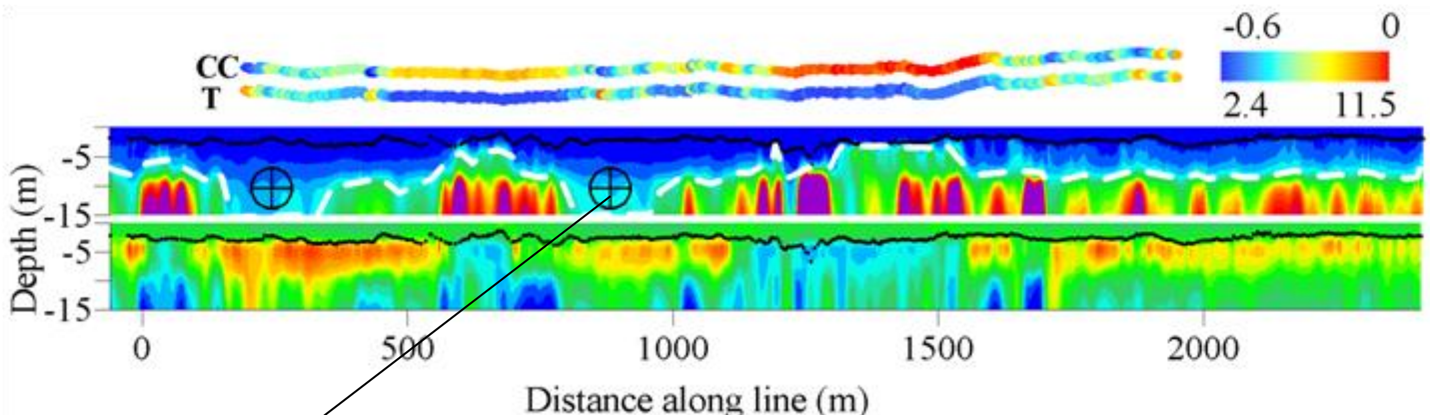
Columbia River at Hanford

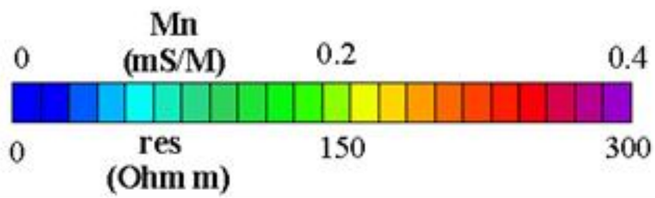
1: Rutgers-Newark; 2: USGS, Office of Groundwater, Branch of Geophysics; 3: Idaho National Laboratory; 4: Pacific Northwest National Laboratory; 5: Lancaster University

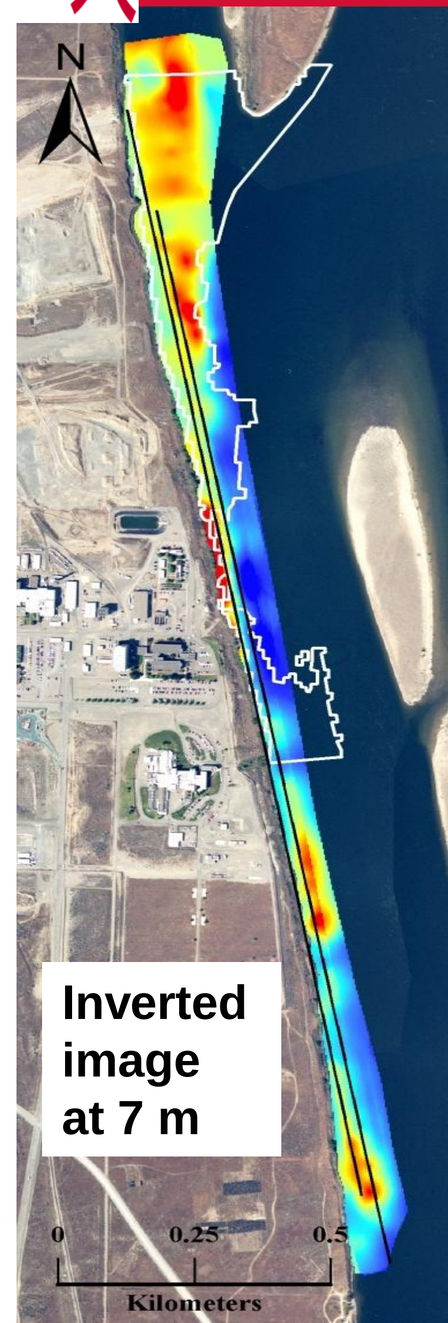
Correlation of DTS and hydrogeologic framework

Focused hyporeheic exchange: temperature anomalies and a correlation between stage and temperature occur where Hanford unit thickest; exchange is muted/absent where Hanford is thin



locally-incised paleochannels?





Line 20 (20 m from shore)

Contaminant Transport at the Hanford Site:

Developing a Conceptual Framework for the Columbia River Corridor

Advanced Simulation Capability for Environmental Management

ASCEM Multi-Lab Program Manager
Paul Dixon

Presentation to Office of Technology Innovation and Development
3rd Quarter Review Meeting July 7-8, 2010

ASCEM National Laboratory Consortium

BERKELEY LAB

Los Alamos NATIONAL LABORATORY EST.1943

Pacific Northwest NATIONAL LABORATORY

OAK RIDGE National Laboratory

SRNL SAVANNAH RIVER NATIONAL LABORATORY

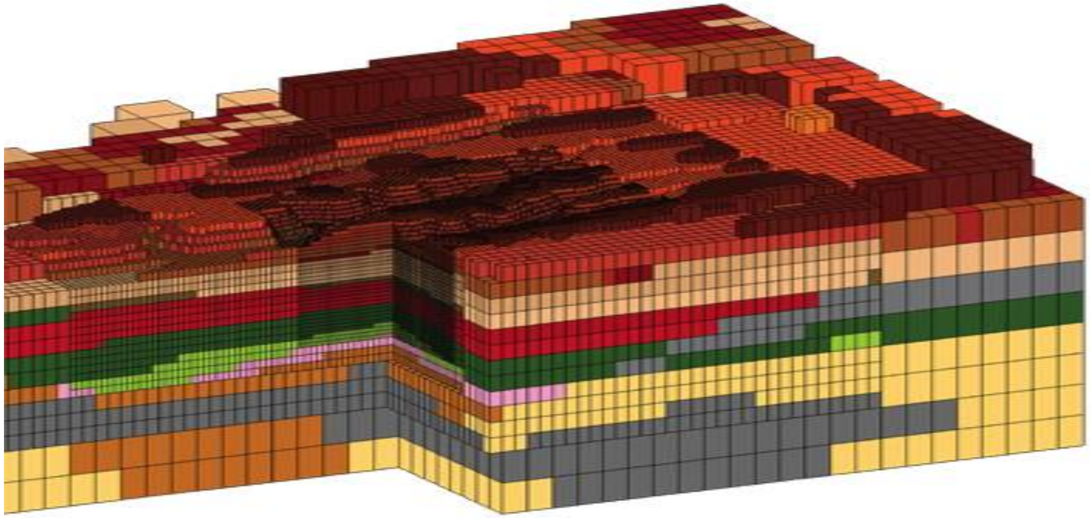
Lawrence Livermore National Laboratory Science in the National Interest

Argonne NATIONAL LABORATORY

INL Idaho National Laboratory

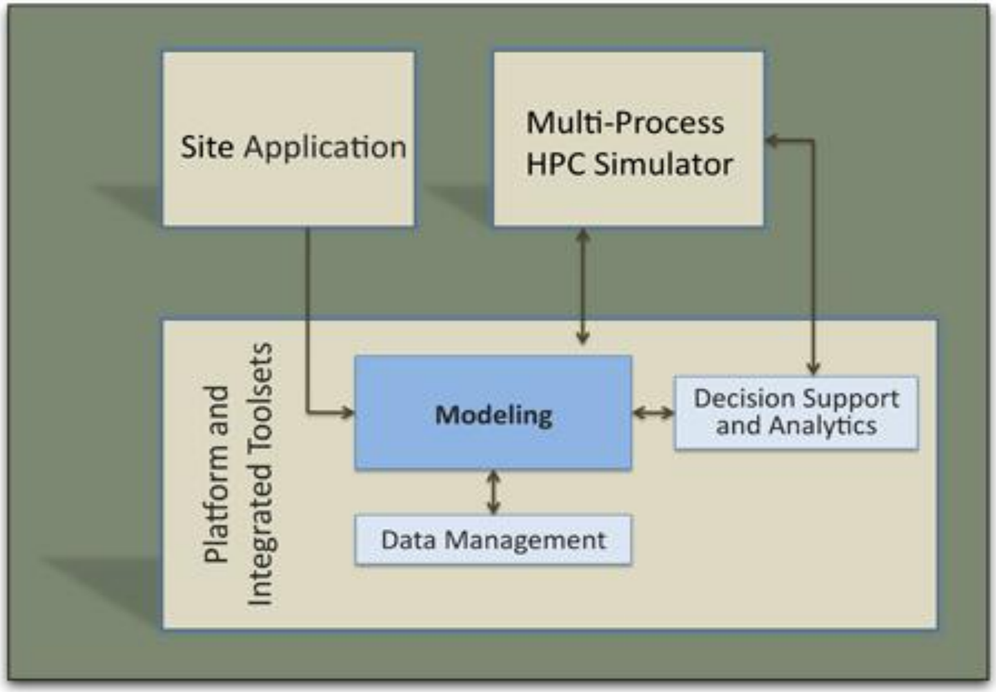
What is ASCEM?

ASCEM is a state-of-the-art ***scientific tool and approach*** *for understanding and predicting contaminant fate and transport in natural and engineered systems. ASCEM is a Modular and open source HPC tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized development of performance and risk assessments for EM cleanup/closure activities* for EM cleanup/closure activities.



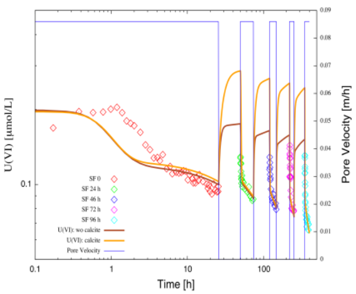
ASCEM

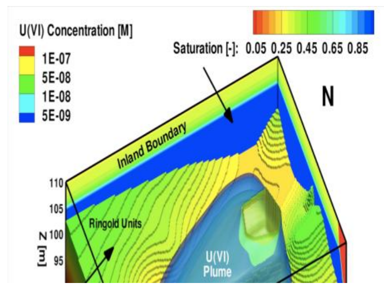
ASCEM Overall Structure



- **Site Applications**
  - Demonstration sites
  - Actively engage site user community to develop and test ASCEM tools
- **Platform and Integrated Toolsets**
  - Facilitate model development and execution, parameter estimation, uncertainty quantification, decision support and risk analysis
- **Multi-Process High Performance Computing Simulator**
  - Modular simulation capability for barrier and waste form degradation, multiphase flow and reactive transport

Multi-Process HPC Simulator



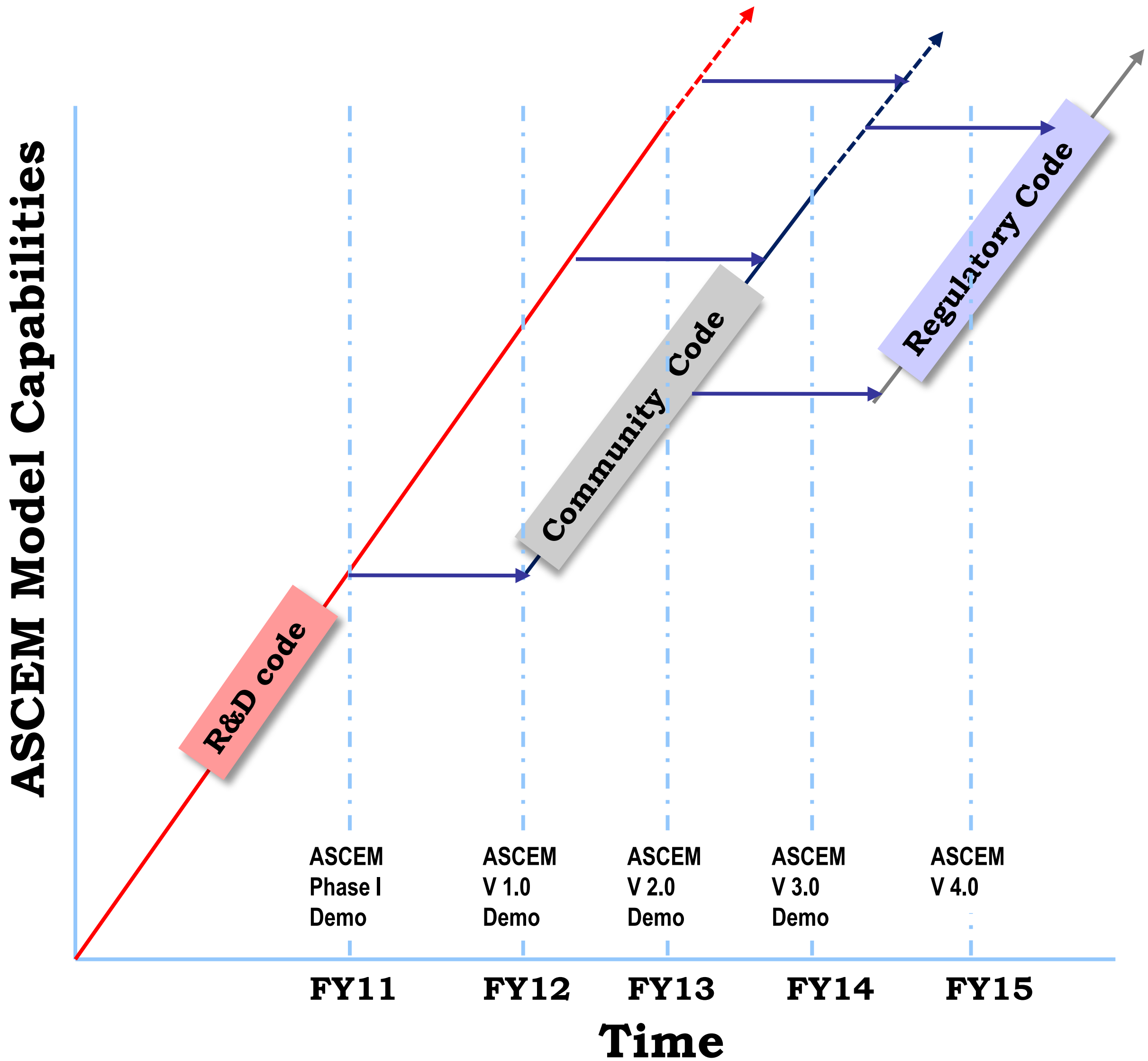


Wide Range of Complexity

Wide Range of Platforms

- Modular HPC simulation capability for waste form and engineered barrier degradation, multiphase flow, and reactive transport
- Efficient, robust simulation from supercomputers to laptops
- Design and build for emerging multi-core and accelerator-based systems
- Open-source project with strong community engagement

ASCEM Software Life Cycle

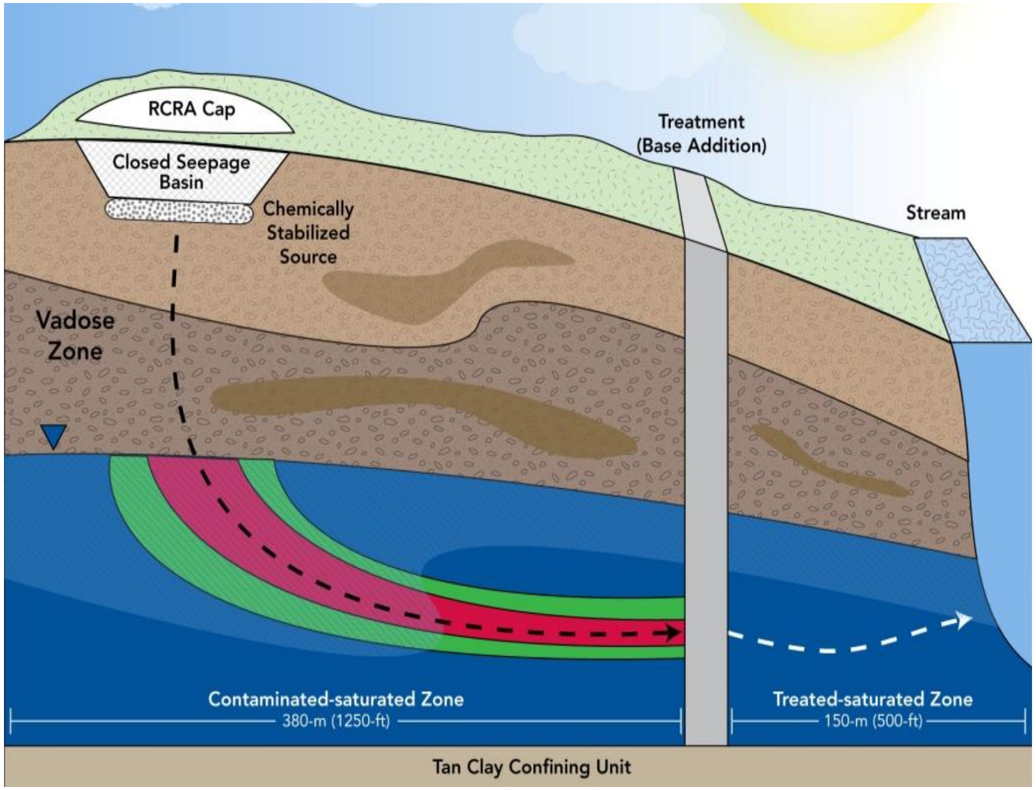


ASCEM

ascemdoe.org

Site Applications Scope

- Provide site data for model development, testing and validation
- Provide sites for demonstrating the platform and HPC simulator
- Establish and maintain interfaces with end users
- Solicit input to requirements specification and development activities



ASCEM

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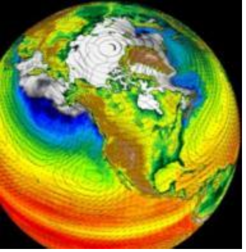


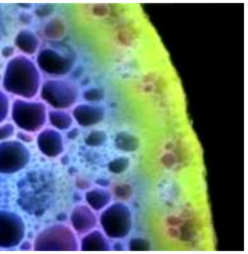
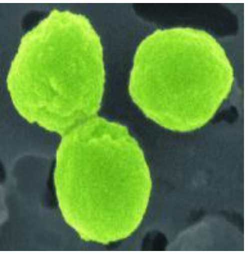

Backup Slides

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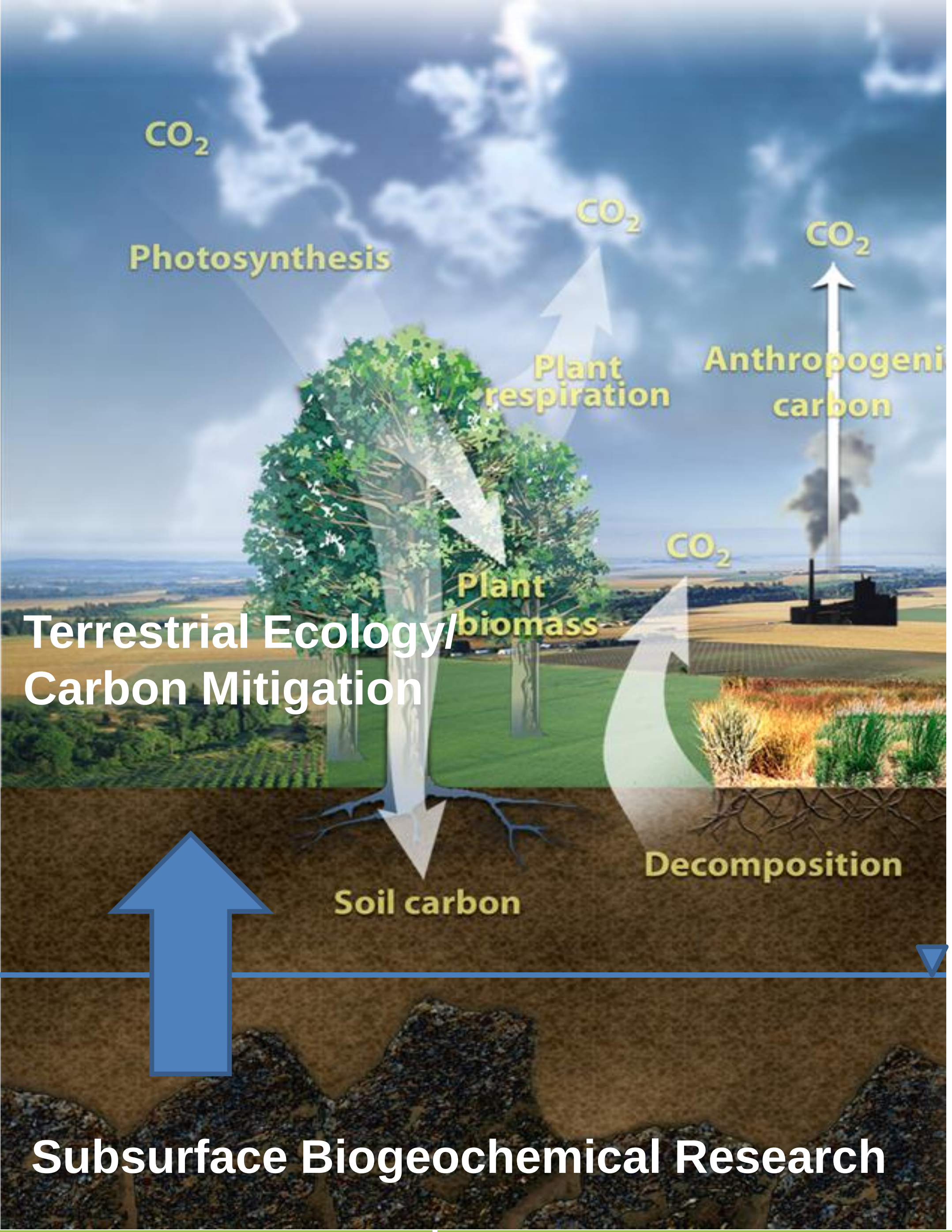
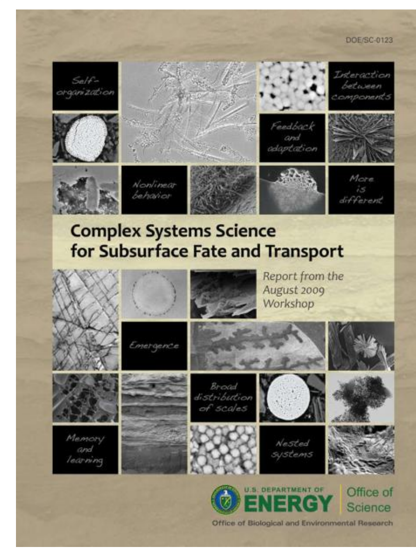


Future Directions

New Strategic Plan for Subsurface Biogeochemical Research

- more integrative within BER
- broadens the applicability of subsurface science
- addresses multiple DOE missions
- looks to integrate with CESD Environmental Systems Science
- informed by a recent workshop "*Complex Systems Science for Subsurface Fate and Transport,* August 2009"



Program Management

Track progress/accomplishment

- Awards, real-world applications
- Website postings of publications (ERSP website and/or the ERSD website) http://www.lbl.gov/ERSP/generalinfo/publications.html

Annual PI meetings (early April each year)

- Mandatory attendance by Lead PIs
- Mandatory poster presentation
- Selected oral presentations

Regular reviews/updates of major program elements

- Quarterly and Annual reports from Field Site lead PIs
- Field Research Executive Committee (FREC)
- Triennial On Site reviews of Lab SFA programs (ORNL, ANL)

Annual progress reports from program projects

- University PIs must submit an annual report for continuation of funding
  - Continued funding subject to program manager approval
- Annual FWP submissions for Labs
  - Continuation subject to program manager approval
- Annual reports from National Lab programs

SBR Long-term PART Measure

Provide sufficient scientific understanding such that DOE sites would be able to incorporate coupled physical, chemical and biological processes into decision making for environmental remediation and long-term stewardship

Progress tracked in the PART process managed by the office of Management and Budget
SBR quarterly PART submissions posted at:
http://esd.lbl.gov/research/projects/ersp/generalinfo/milestones.html

ERSP Science Portfolio

LTM	Strategic Goals	Science Themes	Project Areas	Funding Mechanism
ERSD Long Term Measure Provide sufficient scientific understanding to allow DOE sites to incorporate coupled biological, chemical and physical processes into decision making for environmental remediation	**Goal 1:** Develop an **improved understanding of the processes governing the fate and transport of contaminants in the subsurface** in order to predict and control environmental remediation and long term stewardship of DOE sites.	Fundamental Molecular Scale Research	Surface Chemistry	EMSL, EMSIs Synchrotron support
			Aqueous Complexes	
			Nanoscale Research	
		Subsurface Biogeochemistry	Microbe-Mineral Reactions	ERSP Research: SFA's + Notices
			Contaminant-Mineral Rxns	
		Subsurface Microbiology	Microbial Ecology/Metabolism	
			Microbially Catalyzed Rxns	
		Groundwater Flow and Transport	Aquifer Characterization	
			Groundwater Hydrology	
		Vadose Zone Processes	Geochemical Gradient Rxns	
			Unsaturated Zone Chemistry	
		Conceptual/Computer Model Development	Scaling of Processes	SciDAC
			3D HPC Framework	
		Field Scale Research	Fate & Transport at Well Characterized Field Sites	IFC's
	Goal 2: Explore **new options and concepts for the remediation** of subsurface environments.	Physical/Chemical Remediation Processes	Immobilization	ERSP Research: SFA's + Notices
			Removal Techniques	
			Barrier research	
		Biological Processes	Bioremediation	
		Long Stewardship Research	MNA processes/ Modeling	
	Goal 3: Develop **new measurement and monitoring tools** to better understand and manage contaminant transport.	Site Characterization Technologies	Geophysics Techniques Seismic, GPR, EMT etc.	ERSP Research & SBIR/STTR Projects
		Biological, Chemical and Physical Sensor Technology	Genomics-based techniques	
			Chemical speciation detection	
			Flow detection	
			Autonomous Sampling and Data Collection/Reporting Systems	

http://www.sc.doe.gov/ober/ERSD/Strategic_plan_cover_letter.html

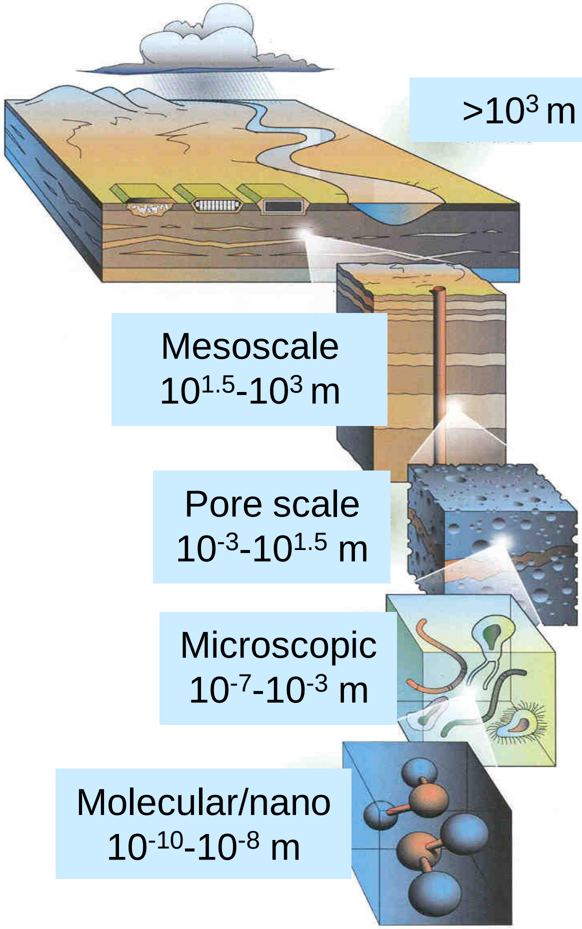
Scientific Focus Areas at the National Laboratories

Team-oriented Approach to Subsurface Science

PNNL ($6.5M) - Integrated investigations of geochemical, microbial and transport processes at different scales. Focus on Hanford Site (U, Tc, Pu)
LBNL ($4.5M) – Integrated investigations of geochemical, microbial and transport processes at different scales. Hanford 100 Area, Old Rifle IFRC, SRS F-Area (U, Cr, I)
ORNL ($3M) – Biogeochemistry, microbial processes (Hg)

ANL ($1.5M) – Synchrotron environmental science
SLAC ($0.7M) – Synchrotron environmental science

LLNL ($1.2M) – Pu geochemistry at NTS – colloid transport
INL ($1.5M) – Immobilization of metal contaminants by amendment-driven mineral precipitation (Sr)



- ***Lab programs rigorously reviewed every three years***
- ***SFA Programs collaborative with the University community***

National Laboratory SFA Research Programs

➢ Argonne National Laboratory	$1.5M
➢ Idaho National Laboratory	$1.2M
➢ Lawrence Berkeley National Laboratory	$4.5M
➢ Lawrence Livermore National Laboratory	$1.2M
➢ Oak Ridge National Laboratory	$3.0M
➢ Pacific Northwest National Laboratory	$6.5M
➢ SLAC National Accelerator Laboratory	$700K

National Laboratory SFA Program Reviews

➢ Argonne National Laboratory	reviewed in 2009
➢ Oak Ridge National Laboratory	reviewed in 2009
➢ Idaho National Laboratory	on-site review in June 2010
➢ Lawrence Berkeley National Laboratory	on-site review in May 2010
➢ Pacific Northwest National Laboratory	review in 2011
➢ SLAC National Accelerator Laboratory	review in 2011
➢ Argonne National Laboratory	review in 2012
➢ Lawrence Livermore National Laboratory	review in 2012
➢ Oak Ridge National Laboratory	review in 2012

U.S. DEPARTMENT OF ENERGY

Office of Science

Program Staffing

Program Manager	Program Responsibilities
Dr. Robert (Todd) Anderson (CESD)	PNNL SFA, SciDAC projects, Notice 08-09 Rifle IFRC, 60 University-led and DOE Lab Co-PI awards
Dr. David Lesmes (CESD)	LBNL SFA, INL SFA, Notice 07-18, Notice LAB 08-30, Hanford IFRC, 57 University-led and DOE Lab Co-PI awards
Mr. Paul Bayer (CESD)	EMSL, ORNL SFA, Oak Ridge IFRC, 12 University-led and DOE Lab Co-PI awards
Dr. Arthur Katz (BSSD)	LLNL SFA, 9 University-led and DOE Lab Co-PI awards
Dr. Roland Hirsch (BSSD)	ANL SFA, SLAC SFA, 8 University-led and DOE Lab Co-PI awards

Basic Research Needs for Geosciences – Relationships to Applied Research Programs

Discovery Research

- Microscopic basis of macroscopic complexity - scaling
- Highly reactive subsurface materials and environments
- Thermodynamics of the solute-to-solid continuum
- Computational geochemistry of complex moving fluids within porous solids
- Integrated analysis, modeling and monitoring of geologic systems
- Simulation of multi-scale systems for ultra-long times

Use-inspired Basic Research

- Mineral-fluid interface complexity and dynamics
- Nanoparticulate and colloid chemistry and physics
- Dynamic imaging of flow and transport
- Transport properties and *in situ* characterization of fluid trapping, isolation and immobilization
- Fluid-induced rock deformation
- Biogeochemical in extreme subsurface environments

Applied Research

- Develop and test methods for assessing storage capacity and for monitoring containment of CO_2 storage
- Develop remediation methods to ensure permanent storage
- Demonstrate procedures for characterizing storage reservoirs and seals
- Integrated models for waste performance prediction and confirmation
- Radionuclide partitioning in repository environments.
- Waste form stability and release models.
- Incorporate new conceptual models into uncertainty assessments.

Technology Maturation & Deployment

- Develop site selection criteria
- Develop storage and operating engineering approaches
- Storage demonstrations
- Apply assessment protocols and technologies for the lifecycle of projects
- Evaluate release of radionuclide inventory from the repository
- Assess corrosion/ alteration of engineered materials
- Long-term safety/risk assessment for emplacement of energy system by-products.

Office of Science

FE, RW, EM, EERE

Geosciences Research Portfolio – 4 Focus Areas

Rock Physics ($4.4M)

- Electrical properties
- Nonlinear elasticity
- Fracturing and imaging
- Signatures of fluids
- Attenuation and scattering
- Electromagnetic inversions
- Time-lapse imaging
- Imaging permeability

Analytical Geochemistry ($4.4M)

- Synchrotron science
- Mass spectrometry
- Isotopic geochemistry

Flow and Transport ($2.1M)

- Channelization
- Fractures
- Porosity evolution
- Large scale transport
- Coupled processes
- Reactive transport
- Thermal-chemical-mechanical feedbacks

Theoretical and Experimental Geochemistry $7.8M)

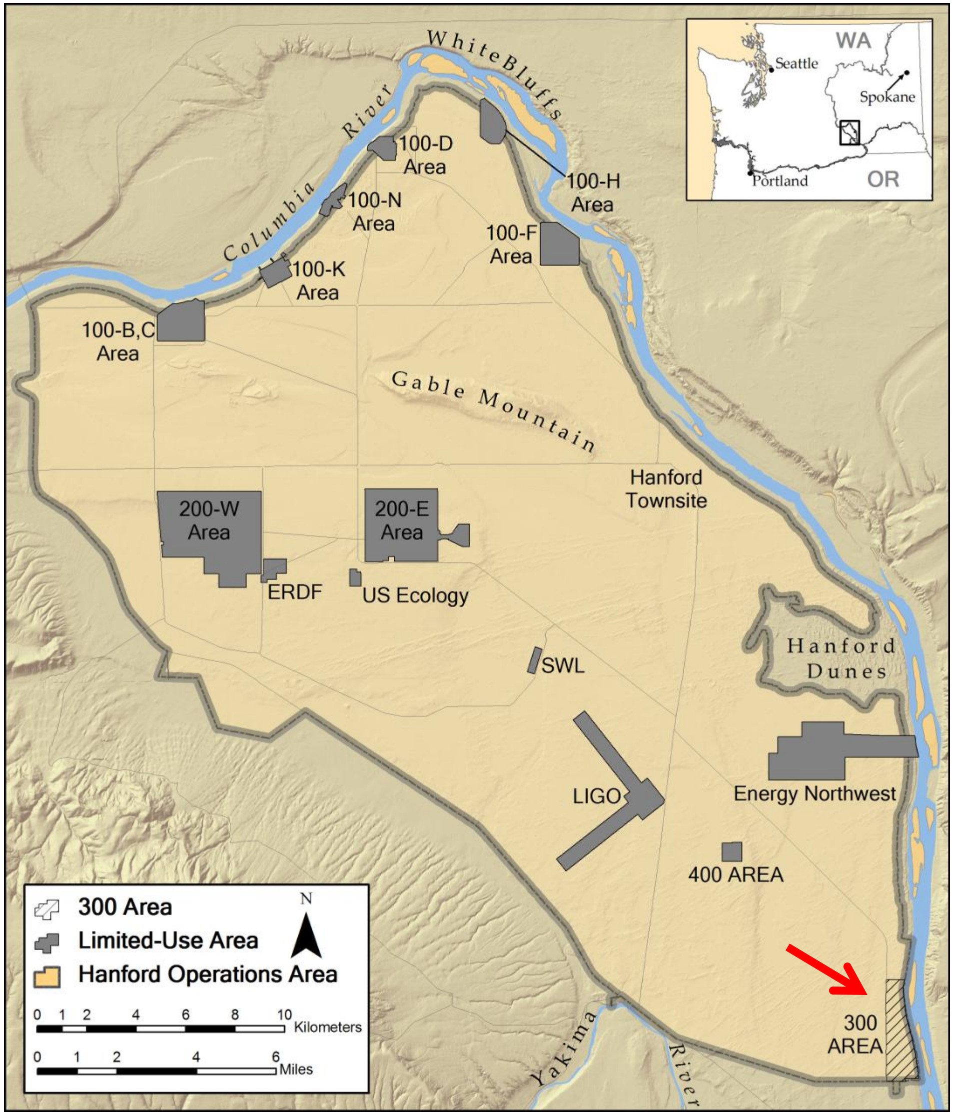
- Computational modeling
- Thermodynamics
- Surface geochemistry
- Reactivity
- Interfacial processes
- Microbial-mineral responses
- Chemical Imaging
- Nanogeosciences

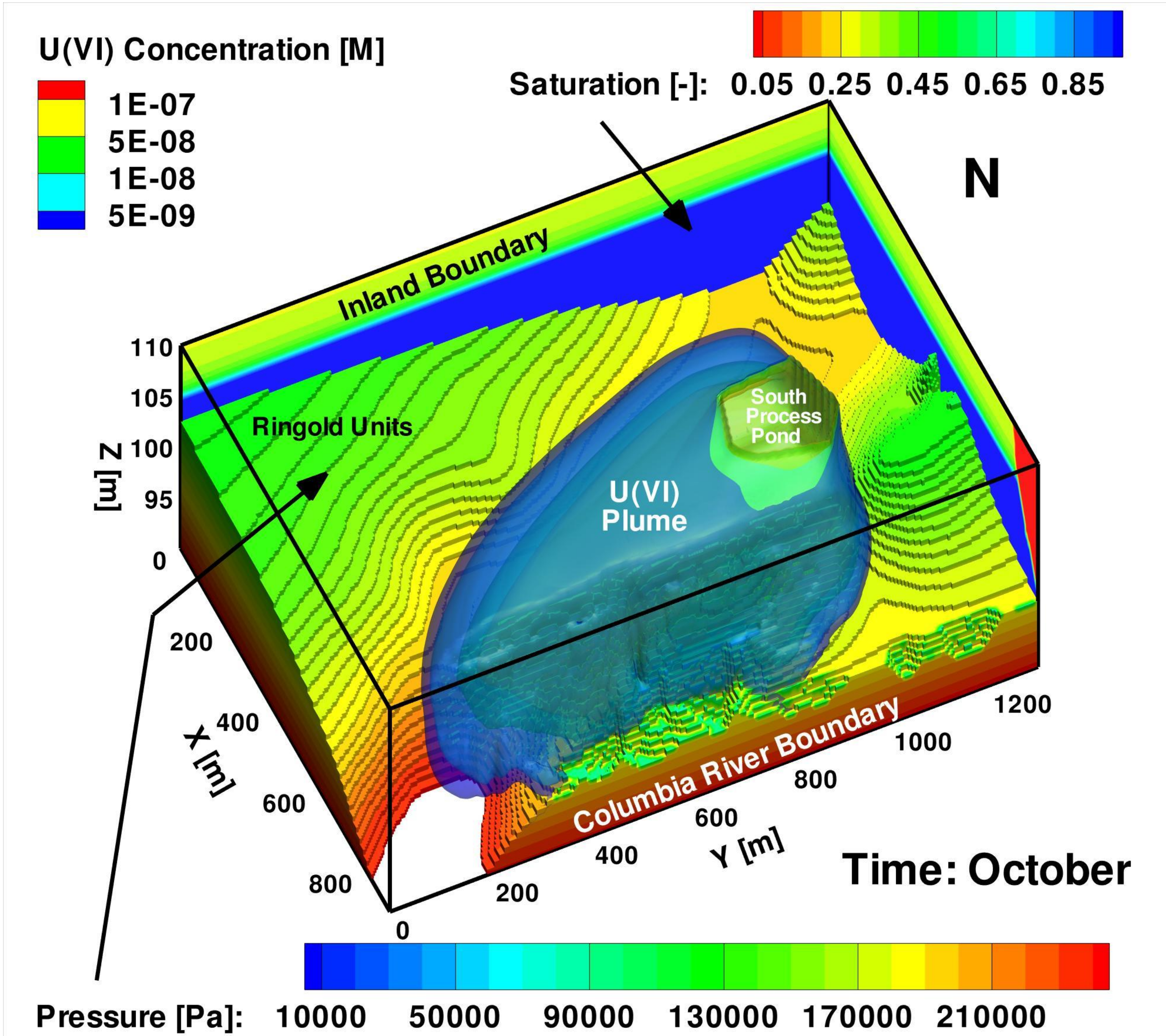
2010: Energy Frontier Research Centers

Single Investigator and Small Group Research

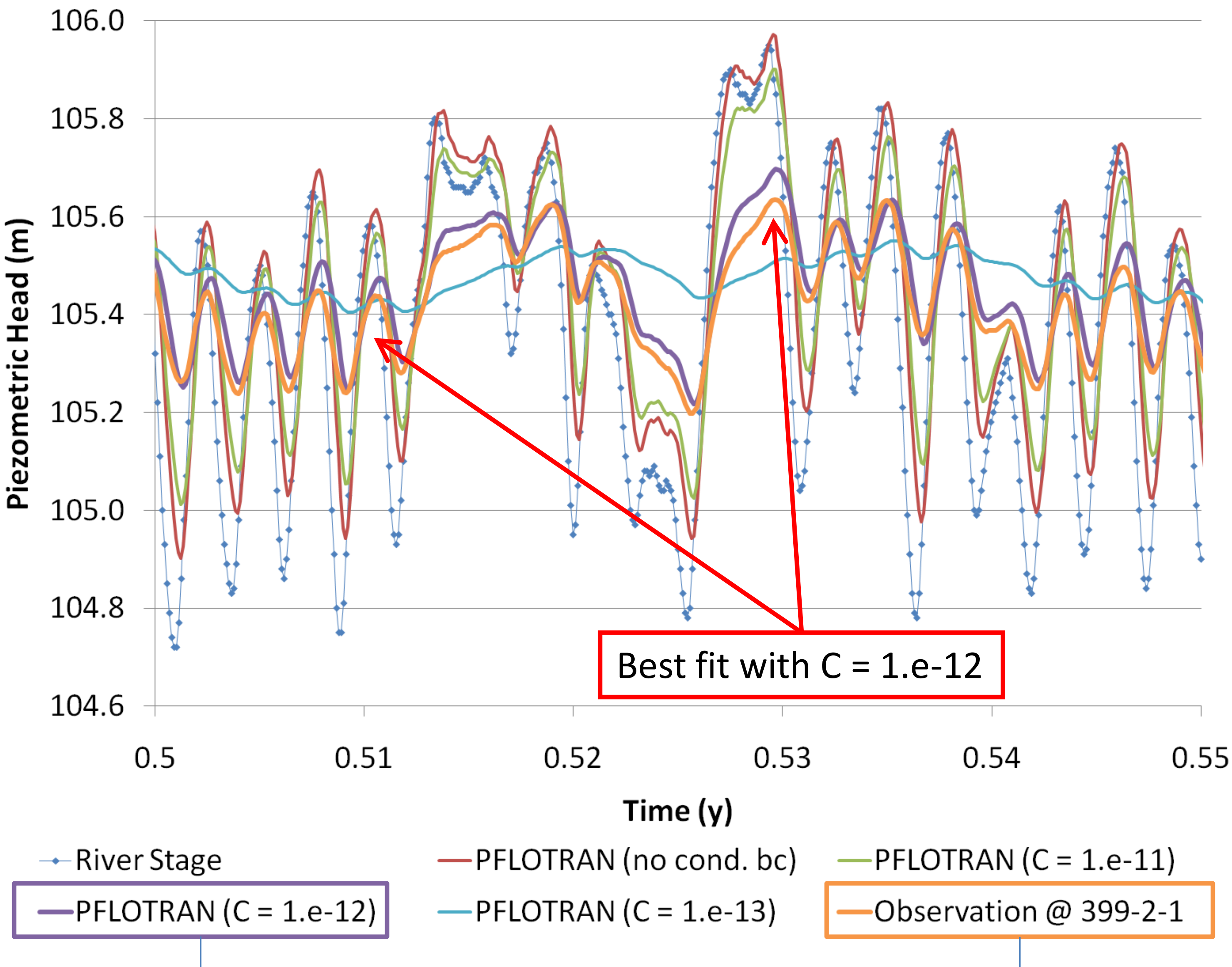
2007 final

Hanford Site

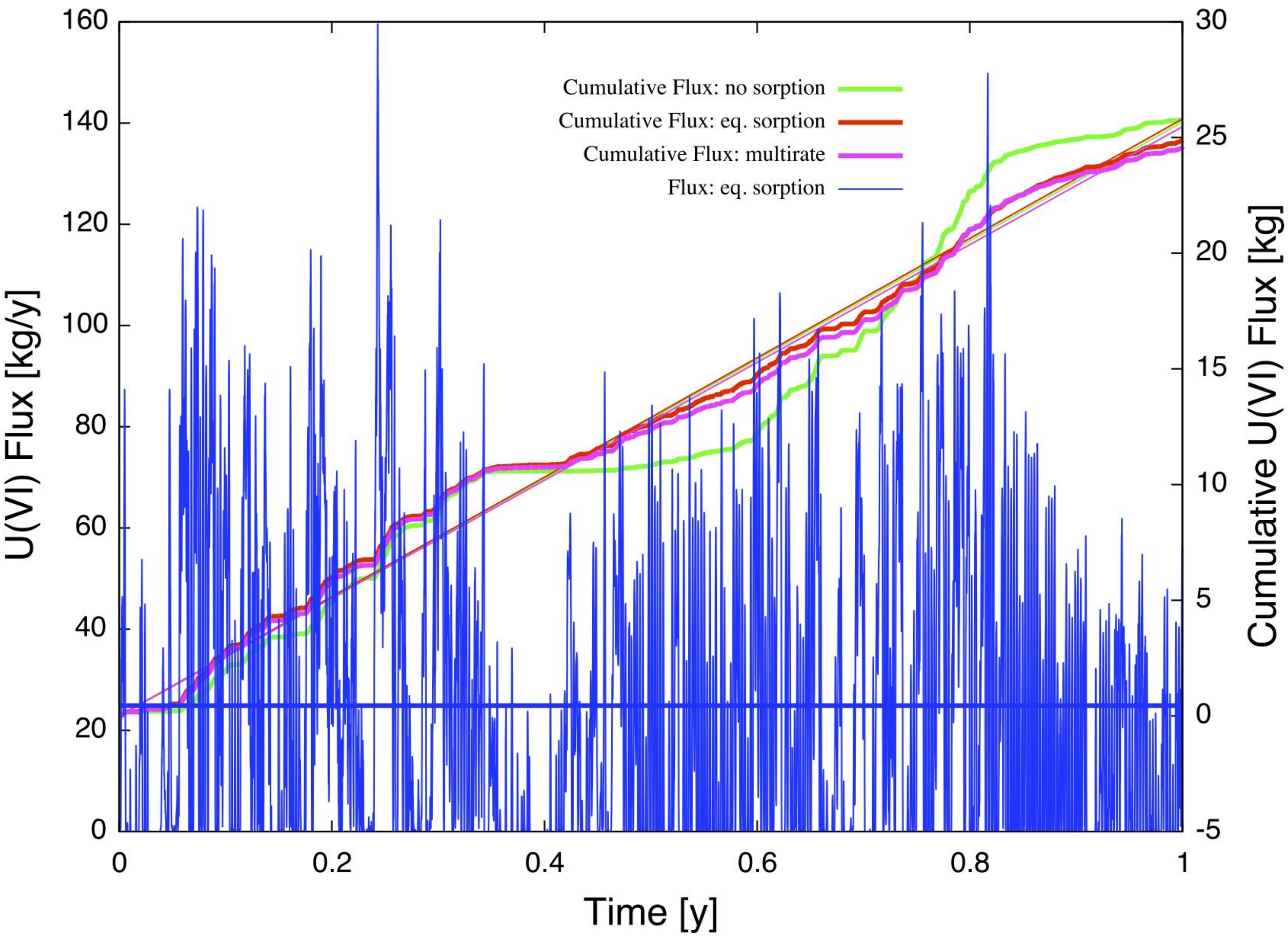



U(VI) Concentration [M]
1E-07
5E-08
1E-08
5E-09
Saturation [-]: 0.05 0.25 0.45 0.65 0.85
N
Inland Boundary
Ringold Units
South Process Pond
U(VI) Plume
Columbia River Boundary
Z [m]
110
105
100
95
0
X [m]
200
400
600
800
Y [m]
0
200
400
600
800
1000
1200
Time: October
Pressure [Pa]: 10000 50000 90000 130000 170000 210000

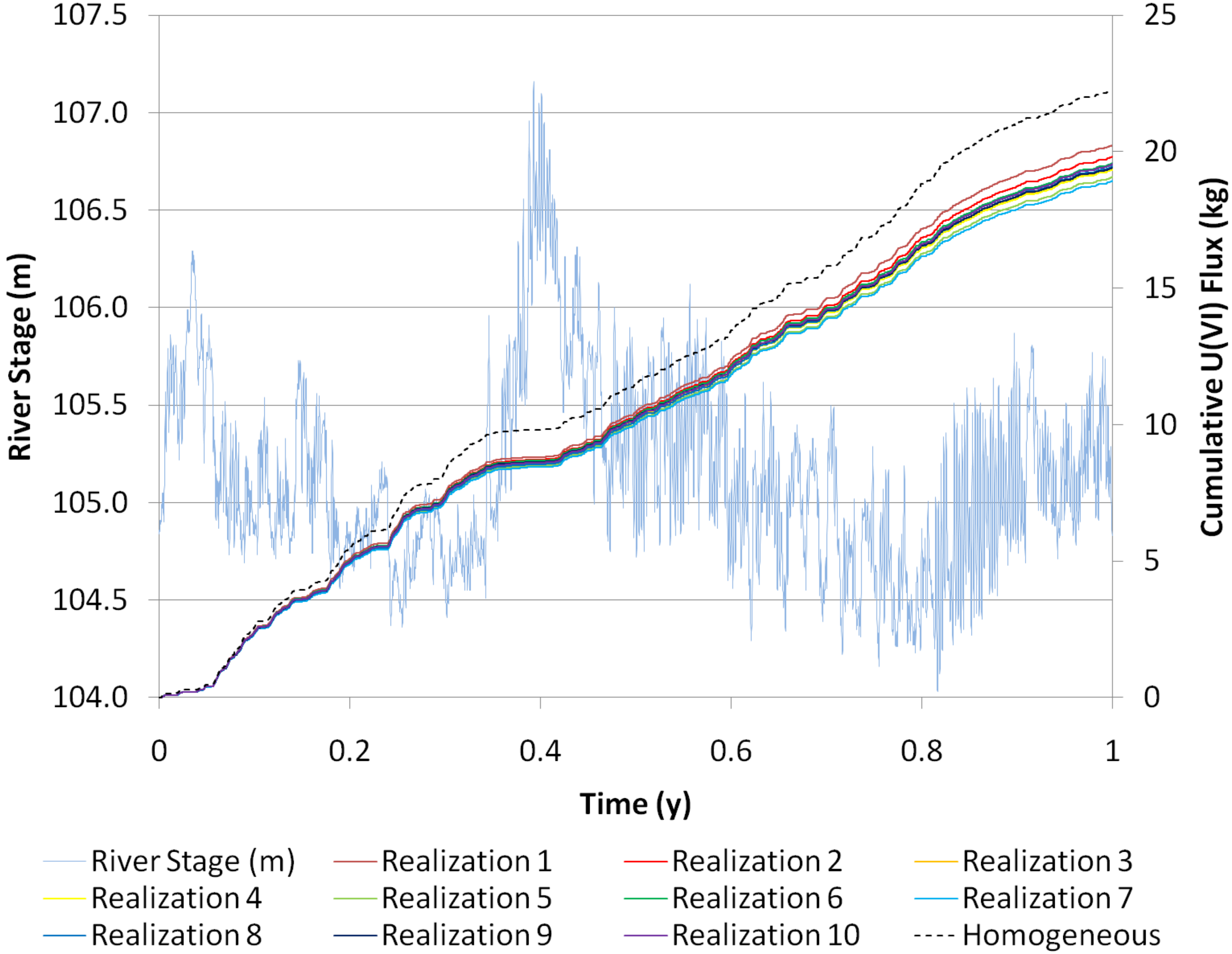
Simulated Piezometric Head as a Function of Conductance Boundary Condition (C)



Comparison of Instantaneous and Cumulative Uranium Flux into the Columbia River



Uranium Flux to Columbia River for 10 Realizations of Random Permeability



Conclusions

- Waterborne IP illuminated the hydrogeologic framework of this major hyporheic corridor
- DTS demonstrates that hydrogeologic framework mapped with IP exerts major control on hyporheic exchange
- Hyporheic exchange is focused, to locations where Hanford formation is thickest, and sometimes co-located with paleochannels